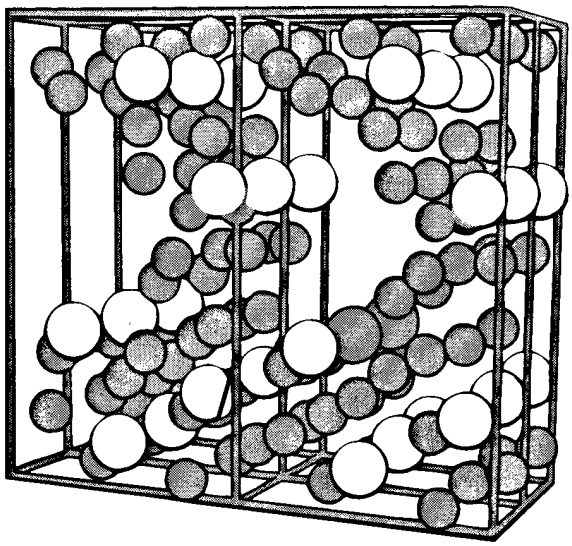
Final Program and Abstracts

SIAM Conference on Mathematical Aspects of

MATERIALS SCIENCE

May 23-26, 2004

Hyatt Regency Los Angeles
at Macy's Plaza
Los Angeles, California



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General Information

SIAM Registration Desk

The SIAM registration desk is located in the Regency Foyer. It is open during the following times:

Saturday, May 22
2:00 PM – 6:00 PM
Sunday, May 23
8:00 AM – 6:30 PM
Monday, May 24
8:00 AM – 5:00 PM
Tuesday, May 25
8:00 AM – 5:00 PM
Wednesday, May 26
8:00 AM – 5:00 PM

Hotel Address

Hyatt Regency Los Angeles at Macy's Plaza
711 South Hope Street
Los Angeles, California 90017

Hotel Telephone Number

The telephone number of Hyatt Regency Los Angeles is (213) 683-1234. The hotel operator can either connect a caller with the SIAM registration desk for a message to be taken and posted to the SIAM message board or forward a caller to an attendee's room to leave a message.

Hotel Check-in and Check-out Times

Check-in time is 3:00 PM
Check-out time is 12:00 PM

General Information

SIAM corporate members provide their employees with knowledge about, access to, and contacts in the applied mathematics and computational sciences community through their membership benefits. Corporate membership is more than just a bundle of tangible products and services; it is an expression of support for SIAM and its programs. SIAM is pleased to acknowledge its corporate members and sponsor. In recognition of their support, non-member attendees who are employed by the following organizations are entitled to the SIAM member registration rate.

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MS04
Program-at-a-Glance

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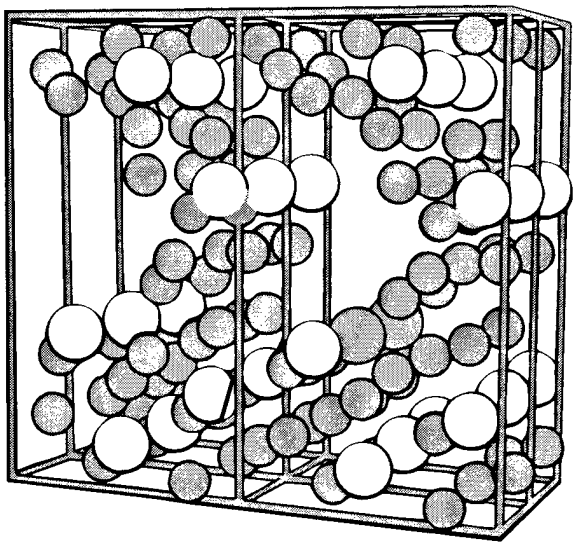


Saturday May 22

2:00 PM - 6:00 PM
Registration Open
Regency Foyer

5:00 PM - 7:00 PM
Welcome Reception
Regency Foyer

Key to abbreviations and symbols

= Coffee breaks

= Lunch breaks

= Poster Session

UNDER CONSTRUCTION:

This program is subject to change. Check the "Program Updates" posted on the bulletin board located in the registration area. Changes are posted once daily, prior to the opening session.

Sunday May 23

8:00 AM - 6:30 PM
Registration Open
Regency Foyer

Internet Cafe
Redondo B

8:15 AM - 8:30 AM
Opening Remarks
Weinan E, Princeton University
Kaushik Bhattacharya, California Institute of Technology
Regency Ballroom A/B

8:30 AM - 9:15 AM
IP1 Orderings on Lattices and the Interfaces between the Domains that Form
John Cahn, National Institute of Standards and Technology
Regency Ballroom A/B

9:15 AM - 10:00 AM
IP2 Stress-Driven Shape Transitions in Solid Films
Brian J. Spencer, State University of New York, Buffalo
Regency Ballroom A/B

10:00 AM - 10:30 AM
Coffee Break
Regency Foyer

10:30 AM - 12:10 PM
Concurrent Sessions
MS1 Composites and Polycrystals: Part I
Regency Ballroom A
MS3 Analytical and Numerical Aspects of Micromagnetics: Part I
Regency Ballroom C
MS4 Computational Modelling of Microstructural Evolution: Part I
Regency Ballroom D
MS5 Superconductivity, Ginzburg-Landau Theory, and Related Topics: Part I
Regency Ballroom E

10:30 AM - 12:35 PM
MS2 Multi-scale Modeling and Simulation of Complex Fluids: Part I
Regency Ballroom B

12:10 PM - 1:30 PM
Lunch
Attendees on their own

1:30 PM - 2:15 PM
IP3 Compatibility and Crystal Microstructure
John Ball, University of Oxford, United Kingdom
Regency Ballroom A/B

2:15 PM - 2:30 PM
Intermission

Sunday May 23

2:30 PM - 4:10 PM
Concurrent Sessions
MS6 Composites and Polycrystals: Part II
Regency Ballroom A
MS7 Multi-scale Modeling and Simulation of Complex Fluids: Part II
Regency Ballroom B
MS8 Analytical and Numerical Aspects of Micromagnetics: Part II
Regency Ballroom C
MS9 Computational Modelling of Microstructural Evolution: Part II
Regency Ballroom D
MS10 Superconductivity, Ginzburg-Landau Theory, and Related Topics: Part II
Regency Ballroom E

4:10 PM - 4:30 PM
Coffee Break
Regency Foyer

4:30 PM - 6:10 PM
Concurrent Sessions
MS11 Composites and Polycrystals: Part III
Regency Ballroom A
MS12 Multi-scale Modeling and Simulation of Complex Fluids: Part III
Regency Ballroom B
MS13 Analytical and Numerical Aspects of Micromagnetics: Part III
Regency Ballroom C
MS14 Computational Modelling of Microstructural Evolution: Part III
Regency Ballroom D
MS15 Superconductivity, Ginzburg-Landau Theory, and Related Topics: Part III
Regency Ballroom E

MS04
Program-at-a-Glance

A Quick Guide to
the SIAM Conference
on Materials Science

OPEN HERE

Tuesday May 25

12:10 PM - 1:30 PM
Lunch
Attendees on their own

1:30 PM - 2:15 PM
IP9 Accelerated Molecular Dynamics Methods
Arthur Voter, Los Alamos National Laboratory
Regency Ballroom A/B

2:15 PM - 2:30 PM
Intermission

2:30 PM - 4:10 PM
Concurrent Sessions
MS40 Contemporary Calculus of Variations for Advanced Materials: Part II
Regency Ballroom A
MS42 Active Materials: Part II
Regency Ballroom C
MS43 Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part II
Regency Ballroom D
MS45 Modes and Resonance in Periodic Structures
Regency Ballroom F

2:30 PM - 4:35 PM
MS41 Multiscale and Stochastic Modeling Methods: Part II
Regency Ballroom B

4:10 PM - 4:30 PM
PP4 Coffee Break and Poster Session IV
Regency Foyer & Manhattan Room

4:30 PM - 6:10 PM
Concurrent Sessions
MS46 Contemporary Calculus of Variations for Advanced Materials: Part III
Regency Ballroom A
MS48 Lattice Models for Materials: Mathematical Results and Open Problems
Regency Ballroom C
MS49 Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part III
Regency Ballroom D
MS50 Long-range Interactions and Microstructure
Regency Ballroom E

4:30 PM - 6:35 PM
MS47 Multiscale and Stochastic Modeling Methods: Part III
Regency Ballroom B

Wednesday May 26

8:00 AM - 5:00 PM
Registration Open
Regency Foyer

Internet Cafe
Redondo B

8:30 AM - 9:15 AM
IP10 Non-Slip vs Slip: The Hydrodynamic Boundary Condition and the Moving Contact Line
Ping Sheng, The Hong Kong University of Science and Technology, Hong Kong
Regency Ballroom A/B

9:15 AM - 10:00 AM
IP11 Liquids, Solids and Elastic Heresy in Between - Is There a 2½th State of Matter?
Mark Warner, Cambridge University, United Kingdom
Regency Ballroom A/B

10:00 AM - 10:30 AM
Coffee Break
Regency Foyer

10:30 AM - 12:10 PM
Concurrent Sessions
MS51 Quantitative Modeling in Biology: Part I
Regency Ballroom A
MS52 Electronic Structure and Atomistic Simulations
Regency Ballroom B
MS53 Challenges in Systems with Nematic and Smectic Order: Part I
Regency Ballroom C
MS54 Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part IV
Regency Ballroom D
MS55 Crack Propagation in Elastic and Viscoelastic Solids: Part I
Regency Ballroom E
MS56 Mathematical Modeling of Electrochemical Systems: Part I
Regency Ballroom F

12:10 PM - 1:30 PM
Lunch
Attendees on their own

Wednesday May 26

1:30 PM - 3:10 PM
Concurrent Sessions
MS57 Quantitative Modeling in Biology: Part II
Regency Ballroom A
MS58 Dynamics of Microstructure and Defects in Solids: Discrete and Continuum Models: Part I
Regency Ballroom B
MS59 Challenges in Systems with Nematic and Smectic Order: Part II
Regency Ballroom C
MS60 Recent Developments in Modeling and Simulations of Interface Problems in Materials Science: Part I
Regency Ballroom E
MS61 Crack Propagation in Elastic and Viscoelastic Solids: Part II
Regency Ballroom D
MS62 Mathematical Modeling of Electrochemical Systems: Part II
Regency Ballroom F

3:10 PM - 3:40 PM
Coffee Break
Regency Foyer

3:40 PM - 5:20 PM
Concurrent Sessions
MS63 Quantitative Modeling in Biology: Part III
Regency Ballroom A
MS64 Dynamics of Microstructure and Defects in Solids: Discrete and Continuum Models: Part II
Regency Ballroom B
MS65 Challenges in Systems with Nematic and Smectic Order: Part III
Regency Ballroom C
MS66 Recent Developments in Modeling and Simulations of Interface Problems in Materials Science: Part II
Regency Ballroom D

5:25 PM
Conference Adjourns

MS04 Program-at-a-Glance

Monday May 24

8:00 AM - 5:00 PM
Registration Open
Regency Foyer

Internet Cafe
Redondo B

8:30 AM - 9:15 AM
IP4 Inverse Design Problems in Electromagnetics and Nano-Photonics
Eli Yablonovitch, University of California, Los Angeles
Regency Ballroom A/B

9:15 AM - 10:00 AM
IP5 Anomalous Light Phenomena with Photonic Crystals
John D. Joannopoulos, Massachusetts Institute of Technology
Regency Ballroom A/B

10:00 AM - 10:30 AM
PP1 Coffee Break and Poster Session I
Regency Foyer & Manhattan Room

Monday May 24

10:30 AM - 12:10 PM
Concurrent Sessions
MS16 Composites and Polycrystals: Part IV
Regency Ballroom A
MS17 Multi-scale Modeling and Simulation of Complex Fluids: Part IV
Regency Ballroom B
MS18 Analytical and Numerical Aspects of Micromagnetics: Part IV
Regency Ballroom C
MS19 Conformal-mapping Methods for Microstructural Evolution
Regency Ballroom D
MS21 Accurate and Efficient Mathematical Methods for Analysis, Design, and Optimization of Photonic Crystal Structures: Part I
Regency Ballroom F

12:10 PM - 1:30 PM
Lunch
Attendees on their own

1:30 PM - 2:15 PM
IP6 Modeling the Mechanical Behavior of Granular Materials
James Jenkins, Cornell University
Regency Ballroom A/B

2:15 PM - 2:30 PM
Intermission

2:30 PM - 4:10 PM
Concurrent Sessions
MS22 Composites and Polycrystals: Part V
Regency Ballroom A
MS23 Multi-scale Modeling and Simulation of Complex Fluids: Part V
Regency Ballroom B
MS24 Ferroelectrical Phenomena in Soft Materials: Part I
Regency Ballroom C
MS25 Modeling and Analysis of Grain Growths in Polycrystalline Materials: Part I
Regency Ballroom D
MS26 Mathematical Modeling and Simulation of Granular Flows: Part I
Regency Ballroom E
MS27 Accurate and Efficient Mathematical Methods for Analysis, Design, and Optimization of Photonic Crystal Structures: Part II
Regency Ballroom F

4:10 PM - 4:30 PM
PP2 Coffee Break and Poster Session II
Regency Foyer & Manhattan Room

Monday May 24

4:30 PM - 6:10 PM
Concurrent Sessions
MS28 Homogenization in Discrete Systems
Regency Ballroom A
MS29 Coarsening Dynamics and Morphology of Faceted Crystal Surfaces Far from Equilibrium
Regency Ballroom B
MS30 Ferroelectrical Phenomena in Soft Materials: Part II
Regency Ballroom C
MS31 Modeling and Analysis of Grain Growths in Polycrystalline Materials: Part II
Regency Ballroom D
MS32 Mathematical Modeling and Simulation of Granular Flows: Part II
Regency Ballroom E
MS33 Light and Wave Propagation in Inhomogeneous Media: Theory and Modeling: Part I
Regency Ballroom F

Tuesday, May 25

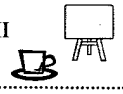
8:00 AM - 5:00 PM
Registration Open
Redondo Foyer

Internet Cafe
Redondo B

8:30 AM - 9:15 AM
IP7 Electron Transport and Dissipation in Nanoscale Devices
Roberto Car, Princeton University
Regency Ballroom A/B

9:15 AM - 10:00 AM
IP8 Rare and Not-So Rare Events in Material Sciences and Beyond
Eric Vanden-Eijnden, Courant Institute of Mathematical Sciences, New York University
Regency Ballroom A/B

10:00 AM - 10:30 AM
PP3 Coffee Break and Poster Session III
Regency Foyer & Manhattan Room



10:30 AM - 12:10 PM
Concurrent Sessions
MS34 Contemporary Calculus of Variations for Advanced Materials: Part I
Regency Ballroom A
MS35 Multiscale and Stochastic Modeling Methods: Part I
Regency Ballroom B
MS36 Active Materials: Part I
Regency Ballroom C
MS37 Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part I
Regency Ballroom D
MS38 Mathematical Modeling and Simulation of Granular Flows: Part III
Regency Ballroom E
MS39 Light and Wave Propagation in Inhomogeneous Media: Theory and Modeling: Part II
Regency Ballroom F

General Information

Funding Agency

SIAM and the Conference Organizing Committee wish to extend their thanks and appreciation to the Office of Naval Research for its support of this conference.

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Visit the membership counter in the registration area during the conference, join online, or download an application at http://www.siam.org/membership/applications.htm, or contact SIAM Customer Service at

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Standard A/V Set-Up in Meeting Rooms

SIAM audio-visual policy as posted on SIAM conference website:

Each plenary session room will have two overhead projectors, two screens, and a data projector. All other breakout rooms will have one overhead projector, one screen, and a data projector.

SIAM is unable to order computers for any speaker. If PowerPoint or another type of electronic presentation is planned, the speaker must bring his/her own computer.

If you have questions regarding availability of equipment in the meeting room of your presentation, please see a SIAM staff member at the registration desk.

E-mail Access

An internet café is available for meeting attendees during registration hours.

Registration Fee Includes

- Welcome Reception
- Admission to poster sessions
- Two coffee breaks daily
- Room set-ups and audio-visual equipment
- Admission to all technical sessions
- Internet café

Job Postings

There is a dedicated bulletin board located in the registration area for job postings. Academic and corporate employers who wish to solicit applications or interview during the conference should post information here. Attendees who wish to review job opportunities should check this board.

Important Notice to Poster Presenters

Poster presenters are requested to set up their poster material in the Regency Foyer and Manhattan rooms. Presenters may set up their posters on May 23 between the hours of 8:00 AM and 6:00 PM. All materials must be posted by 10:00 AM, May 24, the official start time of the session. Posters will remain on display through May 25. Poster displays must be removed by 7:00 PM on May 25. Posters remaining after this time will be discarded. SIAM is not responsible for discarded posters.

Name Badges

Please remember to fill in the emergency contact information on the **back** of your name badge.

Get-togethers

- **Welcome Reception, Saturday, May 22**

- **Poster Sessions**

  Poster sessions are during the coffee breaks

Monday, March 24
10:00 AM - 10:30 AM
4:10 PM - 4:30 PM

Tuesday, March 25
10:00 AM - 10:30 AM
4:10 PM - 4:30 PM

Poster presenters will be with their posters during this time.

Invited Plenary Sessions

**** All Invited Plenary Presentations will take place in the Regency Ballroom A/B****

Sunday, May 23

8:30 AM - 9:15 AM
IP1 Orderings on Lattices and the Interfaces between the Domains that Form
John Cahn, *National Institute of Standards and Technology*

9:15 AM - 10:00 AM
IP2 Stress-Driven Shape Transitions in Solid Films
Brian J. Spencer, *State University of New York, Buffalo*

1:30 PM - 2:15 PM
IP3 Compatibility and Crystal Microstructure
John Ball, *University of Oxford, United Kingdom*

Monday, May 24

8:30 AM - 9:15 AM
IP4 Inverse Design Problems in Electromagnetics and Nano-Photonics
Eli Yablonovitch, *University of California, Los Angeles*

9:15 AM - 10:00 AM
IP5 Anomalous Light Phenomena with Photonic Crystals
John D. Joannopoulos, *Massachusetts Institute of Technology*

1:30 PM - 2:15 PM
IP6 Modeling the Mechanical Behavior of Granular Materials
James Jenkins, *Cornell University*

Invited Plenary Sessions

Tuesday, May 25

8:30 AM - 9:15 AM
IP7 Electron Transport and Dissipation in Nanoscale Devices
Roberto Car, *Princeton University*

9:15 AM - 10:00 AM
IP8 Rare and Not-So Rare Events in Material Sciences and Beyond
Eric Vanden-Eijnden, *Courant Institute of Mathematical Sciences, New York University*

1:30 PM - 2:15 PM
IP9 Accelerated Molecular Dynamics Methods
Arthur Voter, *Los Alamos National Laboratory*

Wednesday, May 26

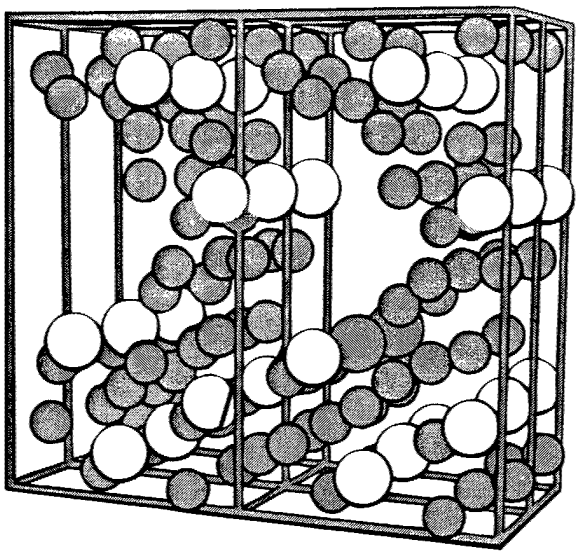
8:30 AM - 9:15 AM
IP10 Non-Slip vs Slip: the Hydrodynamic Boundary Condition and the Moving Contact Line
Ping Sheng, *The Hong Kong University of Science and Technology, Hong Kong*

9:15 AM - 10:00 AM
IP11 Liquids, Solids and Elastic Heresy in Between - Is There a 2½th State of Matter?
Mark Warner, *Cambridge University, United Kingdom*

Final Program

SIAM Conference on Mathematical Aspects of

MATERIALS SCIENCE



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Sunday, May 23

Registration Open
8:00 AM-6:30 PM
Room: Regency Foyer

Internet Cafe
8:00 AM-6:30 PM
Room: Redondo B

Opening Remarks
8:15 AM-8:30 AM
Room: Regency Ballroom A/B

Weinan E, Princeton University

Kaushik Bhattacharya, California Institute of Technology

Sunday, May 23

IP1

Orderings on Lattices and the Interfaces between the Domains that Form

8:30 AM-9:15 AM
Room: Regency Ballroom A/B
Chair: Kaushik Bhattacharya, California Institute of Technology

Gradient systems (large scale ODE) on simple mean field energy functions, constructed to model the behavior chemical species (or scalar spins) on lattices, can reproduce a multitude of ordering phenomena that are observed; a variety of orderings specific to each lattice or lattice complex, and the energies and motions of interfaces between various domains of ordering. These interfaces are anisotropic and show propagation failure at low driving force. Continuizing the discrete lattice formulations to obtain related energy functionals and much-studied PDE retains many of the phenomena, but eliminates the propagation failure and alters the anisotropy.

John Cahn
National Institute of Standards and Technology

Sunday, May 23

IP2

Stress-Driven Shape Transitions in Solid Films

9:15 AM-10:00 AM

Room: Regency Ballroom A/B

Chair: Kaushik Bhattacharya, California Institute of Technology

We present mathematical and experimental aspects of stress-driven morphological transitions occuring in strained solid films. Using a relatively simple continuum model including the effects of surface diffusion, elasticity and surface energy, the morphology of the film can be modeled by a surface evolution equation coupled to elasticity equations in the bulk. From this framework the speaker will discuss the stress-driven instability of planar films, the nonlinear evolution of the instability, and the formation of strained solid drops ("islands" or "quantum dots"). Finally, recent results on the equilibrium shapes of strained solid drops will be highlighted: an asymptotic small-slope theory that gives multiple drop shapes as eigensolutions to a linear integro-differential equation; and numerical work on the influence of anisotropic surface energy that explains the discontinuous droplet shape transitions seen in experiment as a manifestations of a bistable bifurcation diagram for the shape of strained islands.

Brian J. Spencer
State University of New York, Buffalo

Coffee Break

10:00 AM-10:30 AM

Room: Regency Foyer

Sunday, May 23

MS1 (For Part II, see MS6)

Composites and Polycrystals: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom A

The emphasis of the minisymposium will be on effective properties of linear, as well as nonlinear, composites and polycrystals: rigorous homogenization techniques, bounds and estimates, exact relations between various effective physical properties, wave propagation, loss of ellipticity, discrete systems (lattices).

Organizer: Graeme W. Milton
University of Utah

Organizer: Pierre M. Suquet
CNRS, France

10:30-10:50 Bounds for Conducting Networks
Andrea Braides, University of Rome, Italy

10:55-11:15 The G-closure Problem: The Geometric Approach
Yury Grabovsky and Omar Hijab, Temple University

11:20-11:40 New Exact Results for the Effective Electric, Elastic, Piezoelectric and other Properties of Composite Ellipsoid Assemblages
Yakov Benveniste, University of Tel Aviv, Israel and Graeme G. Milton, University of Utah

11:45-12:05 Cross Properties for Multiphase Composites
Vincenzo Nesi, and Enrico Rogora, Universitá di Roma I, Italy

Sunday, May 23

MS2 (For Part II, see MS7)

Multi-scale Modeling and Simulation of Complex Fluids: Part I

10:30 AM-12:35 PM

Room: Regency Ballroom B

Complex fluids are materials exhibiting both fluid and non-fluid like behavior, which encompass solutions and melts of polymers, nanocomposites, liquid crystals, forms, emulsions, gels, and many biomaterials etc. Many fascinating and intriguing phenomena have been reported in flows of complex fluids, which are often related to effects of multiple spatial and time scales as well as the coupling between the macroscopic flow and materials' micro-structures. Modeling and simulation of complex fluids have been a challenge for the scientific community over the year.

Recently, mathematics community has become more and more involved in research on these fascinating materials. The goal of the symposium at the meeting is to bring together researchers from different disciplines and different continents to exchange ideas and forge new collaborations to tackle issues in modeling and simulation of complex fluids.

Organizer: Claude Le Bris
CERMICS ENPC, France

Organizer: Chun Liu
Pennsylvania State University

Organizer: Qi Wang
Florida State University

Organizer: Pingwen Zhang
Peking University, China

10:30-10:50 A Mathematical Overview on Micro-macro Models for Complex Fluids
Claude Le Bris, ENPC/CERMICS, France

10:55-11:15 Moment Closure and Numerical Simulations of a Complex Fluid Model
Qiang Du, Chun Liu, and *Peng Yu*, Pennsylvania State University

11:20-11:40 Numerical Analysis of Polymeric Fluid Flows
Tony Lelievre, CERMICS ENPC, France

11:45-12:05 Some Theoretical Results for the Dumbbell Model of Polymeric Fluids
Tiejun Li, Peking University, China

12:10-12:30 Ferroelectric Phases of Chiral Smectic C Liquid Crystals
Maria-Carme Calderer, University of Minnesota and Qi Wang, Florida State University

Sunday, May 23

MS3 (For Part II, see MS8)

Analytical and Numerical Aspects of Micromagnetics: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom C

The micromagnetic variational principle is a nonconvex variational problem whose local minima represent the stable magnetization patterns of a ferromagnetic body. The associated evolution, Landau-Lifshitz-Gilbert dynamics, describes magnetic switching and the response of a ferromagnet to a varying applied field. These models capture the remarkable multiscale complexity of magnetic materials. Their analysis and simulation raises fundamental and challenging issues of physics and mathematics. Current issues include: the identification of simpler reduced models in physically-relevant asymptotic regimes; the question whether solutions develop singularities; the analysis and simulation of thermally-activated switching pathways; and development of more efficient and accurate numerical schemes.

Organizer: Robert V. Kohn
Courant Institute of Mathematical Sciences, New York University

10:30-10:50 Finite-Temperature Micromagnetic Simulations of Magnetization Reversal
Greg Brown, Oak Ridge National Laboratory

10:55-11:15 Motion of Magnetic Domain Walls in Thin, Narrow Strips
Michael Donahue and Donald Porter, National Institute of Standards and Technology

11:20-11:40 Micromagnetic Simulations of Demagnetization Curves for the Nanocrystalline PrFeB Magnets
Xiao-Ping Wang, Hong Kong University of Science and Technology, Hong Kong

11:45-12:05 Micromagnetics Simulations in Multilayers
Carlos Garcia-Cervera, University of California, Santa Barbara

Sunday, May 23

MS4 (For Part II, see MS9)

Computational Modelling of Microstructural Evolution: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom D

Microstructures have a key role in determining properties of materials. Thus, understanding their evolution during processing or operation is necessary in achieving desired material properties and optimized performance. The recent advances in numerical methods and computational power have provided a fertile ground for computational investigations to flourish in this traditionally experimental field, and models and simulations are becoming more and more accurate and robust. In this mini-symposium, we gather researchers utilizing various modelling methods. In particular, we bring together both view points from the sharp interface and diffuse interface methods, as well as those of experimental work.

Organizer: Katsuyo Thornton
Northwestern University

Organizer: Peter Voorhees
Northwestern University

10:30-10:50 Computational Modelling of Microstructure Evolution
Katsuyo Thornton and P. W. Voorhees, Northwestern University; Geoffrey McFadden, Julia Slutsker, and James Warren, National Institute of Standards and Technology; and Alex Roytburd, University of Maryland

10:55-11:15 Analytical and Numerical Methods for Studying Phase Transformations in Compositionally Stressed Thin Films
Perry Leo, and Yubao Zhen, University of Minnesota

11:20-11:40 Phase-field Modeling of Morphological Evolution in Thin Films
Long-Qing Chen, S Y. Hu, and D J. Seol, Pennsylvania State University

11:45-12:05 Three-Dimensional Simulations of the Early Stages of SiGe Quantum Dot Growth
Vivek Shenoy and *Ashwin Ramasubramaniam*, Brown University

Sunday, May 23

MS5 (For Part II, see MS10)

Superconductivity, Ginzburg-Landau Theory, and Related Topics: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom E

With the recent award of the Nobel Prize in Physics, a renewed attention has been focused on theoretical foundations of superconductivity and superfluidity. The award recognizes Ginzburg-Landau theory as "being of great importance in physics ...". The speakers in this minisymposium will describe their recent research in Ginzburg-Landau theory and related phenomena including: (1) the development or refinement of mezoscale and macroscale models for quantized vortices; (2) mathematical aspects of the Ginzburg-Landau theory and applications in the practical study of dynamics of vortices in superconductivity, superfluidity, and in problems describing defects in liquid crystals; (3) numerical studies of the vortex phenomena.

Organizer: Qiang Du
Pennsylvania State University

Organizer: Leonid Berlyand
Pennsylvania State University

Organizer: Dmitry Golovaty
University of Akron

10:55-11:15 Ginzburg-Landau Minimizers with Prescribed Degrees in Perforated Domains. Capacity of the Domain and Emergence of Vortices
Leonid Berlyand, Pennsylvania State University and Petru Mironescu, Universite de Paris-Sud, France

11:20-11:40 Ginzburg-Landau Models on Thin Spherical Shells
Qiang Du, Pennsylvania State University and *Lili Ju*, University of Minnesota

11:45-12:05 The Bifurcation of Periodic Solutions of the Ginzburg-Landau Equations near a flat wall
Yaniv Almog, Israel Institute of Technology, Israel

10:30-10:50 Vortex Filaments in Bose-Einstein Condensates
Robert Jerrard, University of Toronto, Canada

Lunch

12:10 PM-1:30 PM

Attendees on their own

Sunday, May 23

IP3

Compatibility and Crystal Microstructures

1:30 PM-2:15 PM

Room: Regency Ballroom A/B

Chair: Weinan E, Princeton University

The lecture will describe various ideas related to compatibility and incompatibility of gradients that provide information concerning the formation and morphology of martensitic microstructures in single crystals and polycrystals. From a mathematical perspective this involves consideration of the structure of gradient Young measures, the quasiconvexity condition of the multi-dimensional calculus of variations, quasiregular maps, and generalizations of the Hadamard jump condition. A typical question is whether in a given experimental situation complex microstructures such as those involving layers within layers are preferred to simpler ones.

John Ball
University of Oxford, United Kingdom

Intermission

2:15 PM-2:30 PM

Sunday, May 23

MS6 (For Part I, see MS1)

Composites and Polycrystals: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom A

The emphasis of the minisymposium will be on effective properties of linear, as well as nonlinear, composites and polycrystals: rigorous homogenization techniques, bounds and estimates, exact relations between various effective physical properties, wave propagation, loss of ellipticity, discrete systems (lattices).

Organizer: Graeme W. Milton
University of Utah

Organizer: Pierre M. Suquet
CNRS, France

2:30-2:50 Higher-order Bounds for Constitutive Relations of Nonlinear Composites
John Willis, University of Cambridge, United Kingdom

2:55-3:15 Self-consistent Variational Approach to Anisotropic Nonlinear Conducting
Yves P. Pellegrini and Francois Willot, CEA, France and Martin Idiart and Pedro Ponte Castaneda, University of Pennsylvania

3:20-3:40 Perfectly Plastic Heterogeneous Materials
Guillermo Goldsztein, Georgia Institute of Technology

3:45-4:05 The Influence of Fluctuations in Volume Fraction on the Effective Properties of Nonlinear Composites
Pierre M. Suquet, CNRS, France

Sunday, May 23

MS7 (For Part I, see MS21) (For Part III, see MS12)

Multi-scale Modeling and Simulation of Complex Fluids: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom B

Complex fluids are materials exhibiting both fluid and non-fluid like behavior, which encompass solutions and melts of polymers, nanocomposites, liquid crystals, forms, emulsions, gels, and many biomaterials etc. Many fascinating and intriguing phenomena have been reported in flows of complex fluids, which are often related to effects of multiple spatial and time scales as well as the coupling between the macroscopic flow and materials' micro-structures. Modeling and simulation of complex fluids have been a challenge for the scientific community over the year.

Recently, the mathematics community has become more and more involved in research on these fascinating materials. The goal of the symposium at the meeting is to bring together researchers from different disciplines and different continents to exchange ideas and forge new collaborations to tackle issues in modeling and simulation of complex fluids.

Organizer: Claude Le Bris
CERMICS ENPC, France

Organizer: Chun Liu
Pennsylvania State University

Organizer: Qi Wang
Florida State University

Organizer: Pingwen Zhang
Peking University, China

2:30-2:50 Multiscale Approach to Flows of Liquid Crystal Polymers
Qi Wang, Florida State University

2:55-3:15 Flow-induced Structures and Property Relationships in Nano-composite
M. Greg Forest, University of North Carolina, Chapel Hill

3:20-3:40 Diffuse-interface Simulations of Two-phase Flows of Complex Fluids
Jimmy Feng, University of British Columbia, Canada

3:45-4:05 Adaptive Mesh Refinement for Complex Fluids
Mark Sussman and Qi Wang, Florida State University

Sunday, May 23

MS8 (For Part III, see MS13)

Analytical and Numerical Aspects of Micromagnetics: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom C

The micromagnetic variational principle is a nonconvex variational problem whose local minima represent the stable magnetization patterns of a ferromagnetic body. The associated evolution, Landau-Lifshitz-Gilbert dynamics, describes magnetic switching and the response of a ferromagnet to a varying applied field. These models capture the remarkable multiscale complexity of magnetic materials. Their analysis and simulation raises fundamental and challenging issues of physics and mathematics. Current issues include: the identification of simpler reduced models in physically-relevant asymptotic regimes; the question whether solutions develop singularities; the analysis and simulation of thermally-activated switching pathways; and development of more efficient and accurate numerical schemes.

Organizer: Robert V. Kohn
Courant Institute of Mathematical Sciences, New York University

2:30-2:50 Numerical Methods for the Micromagnetic Simulation of the Entire Recording Process
Thomas Schrefl, Technische Universitat Vienna, Austria

2:55-3:15 2-D Stability of Néel Walls
Hans Knuepfer, University of Bonn, Germany

3:20-3:40 A New Regime for Critical Fields
Ruben Cantero-Alvarez, University of Bonn, Germany

3:45-4:05 Simulating Ferromagnetic Nanostructures with Finite Elements
Riccardo Hertel, Max Planck Institute, Halle, Germany

Sunday, May 23

MS9 (For Part III, see MS14)

Computational Modelling of Microstructural Evolution; Part II

2:30 PM-4:10 PM

Room: Regency Ballroom D

Microstructures have a key role in determining properties of materials. Thus, understanding their evolution during processing or operation is necessary in achieving desired material properties and optimized performance. The recent advances in numerical methods and computational power have provided a fertile ground for computational investigations to flourish in this traditionally experimental field, and models and simulations are becoming more and more accurate and robust. In this mini-symposium, we gather researchers utilizing various modelling methods. In particular, we bring together both view points from the sharp interface and diffuse interface methods, as well as those of experimental work.

Organizer: Katsuyo Thornton
Northwestern University

Organizer: Peter Voorhees
Northwestern University

2:30-2:50 Microstructure and Coarsening Kinetics of Ordered Precipitates in Ni-Base Alloys: Comparison between Experimental Results and Modeling
Alan J. Ardell, University of California, Los Angeles

2:55-3:15 Phase Field Modeling: A Quantitative Application to Phase Transformations in Ni-based Superalloys
Alphonse Finel, ONERA, France and Yann M. Le Bouar, CNRS, France

3:20-3:40 The Role of Heterogeneities in Solidification: A Dirt-dynamics Duality
James Warren, National Institute of Standards and Technology

3:45-4:05 Nucleation in Phase Field Methods
Yann M. Le Bouar, and Alphonse Finel, CNRS, France

Sunday, May 23

MS10 (For Part III, see MS15)

Superconductivity, Ginzburg-Landau Theory, and Related Topics: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom E

With the recent award of the Nobel Prize in Physics, a renewed attention has been focused on theoretical foundations of superconductivity and superfluidity. The award recognizes Ginzburg-Landau theory as "being of great importance in physics ..". The speakers in this minisymposium will describe their recent research in Ginzburg-Landau theory and related phenomena including: (1) the development or refinement of mezoscale and macroscale models for quantized vortices; (2) mathematical aspects of the Ginzburg-Landau theory and applications in the practical study of dynamics of vortices in superconductivity, superfluidity, and in problems describing defects in liquid crystals; (3) numerical studies of the vortex phenomena.

Organizer: Qiang Du
Pennsylvania State University

Organizer: Leonid Berlyand
Pennsylvania State University

Organizer: Dmitry Golovaty
University of Akron

2:30-2:50 Vortices in the Ginzburg-Landau Model of Superconductivity in the Large Kappa Limit
Sylvia Serfaty, Courant Institute of Mathematical Sciences, New York University

2:55-3:15 Surface Superconductivity of Type II Superconductors in 3 Dimensions
Xingbin Pan, National University of Singapore, Republic of Singapore

3:20-3:40 Location and Bending of Vortex Lines in Three Dimensional Domains
Michal Kowalczyk, Kent State University

3:45-4:05 Fractional Degree Vortices for a Spin-coupled Ginzburg-Landau System
Stanley Alama and Lia Bronsard, McMaster University, Canada

Coffee Break

4:10 PM-4:30 PM

Room: Regency Foyer

Sunday, May 23

MS11 (For Part IV, see MS16)

Composites and Polycrystals: Part III

4:30 PM-6:10 PM

Room: Regency Ballroom A

The emphasis of the minisymposium will be on effective properties of linear, as well as nonlinear, composites and polycrystals: rigorous homogenization techniques, bounds and estimates, exact relations between various effective physical properties, wave propagation, loss of ellipticity, discrete systems (lattices).

Organizer: Graeme W. Milton
University of Utah

Organizer: Pierre M. Suquet
CNRS, France

4:30-4:50 Stability of Composite Materials with Inclusions of Negative Stiffness
Roderick Lakes and Y.C. Wang, University of Wisconsin, Madison

4:55-5:15 Homogenization and Stability in Nonlinear Solids with Periodic and Almost Periodic Microstructures
Nicholas Triantafyllidis, University of Michigan

5:20-5:40 Effective Behavior, Field Fluctuations and Loss of Ellipticity in Hyperelastic Composites
Pedro Ponte Castaneda and Oscar Lopez Pamies, University of Pennsylvania

5:45-6:05 Propagation and Lozalisation of Waves in High Contrast Periodic Media and Photonic Crystals
Valery Smyshlyaev, University of Bath, United Kingdom

Sunday, May 23

MS12 (For Part IV, see MS17)

Multi-scale Modeling and Simulation of Complex Fluids: Part III

4:30 PM-6:10 PM

Room: Regency Ballroom B

Complex fluids are materials exhibiting both fluid and non-fluid like behavior, which encompass solutions and melts of polymers, nanocomposites, liquid crystals, forms, emulsions, gels, and many biomaterials etc. Many fascinating and intriguing phenomena have been reported in flows of complex fluids, which are often related to effects of multiple spatial and time scales as well as the coupling between the macroscopic flow and materials' micro-structures. Modeling and simulation of complex fluids have been a challenge for the scientific community over the year.

Recently, the mathematics community has become more and more involved in research on these fascinating materials. The goal of the symposium at the meeting is to bring together researchers from different disciplines and different continents to exchange ideas and forge new collaborations to tackle issues in modeling and simulation of complex fluids.

Organizer: Chun Liu
Pennsylvania State University

Organizer: Qi Wang
Florida State University

Organizer: Pingwen Zhang
Peking University, China

Organizer: Claude Le Bris
ENPC/CERMICS, France

4:30-4:50 On Multiscale Effects in Viscoelaticity
Chun Liu, Pennsylvania State University

4:55-5:15 Dynamics of Ferroelectric Phases of Liquid Crystals
M. Carme Calderer, University of Minnesota

5:20-5:40 Numerical Modeling of Periodic Structures in Liquid Crystal Films
Eugene Gartland, Kent State University

5:45-6:05 Accurate Numerical Simulations of Nematic Polymers in Shear Flow using
Ruhai Zhou, University of North Carolina

Sunday, May 23

MS13 (For Part IV, see MS18)

Analytical and Numerical Aspects of Micromagnetics: Part III

4:30 PM-6:10 PM

Room: Regency Ballroom C

The micromagnetic variational principle is a nonconvex variational problem whose local minima represent the stable magnetization patterns of a ferromagnetic body. The associated evolution, Landau-Lifshitz-Gilbert dynamics, describes magnetic switching and the response of a ferromagnet to a varying applied field. These models capture the remarkable multiscale complexity of magnetic materials. Their analysis and simulation raises fundamental and challenging issues of physics and mathematics. Current issues include: the identification of simpler reduced models in physically-relevant asymptotic regimes; the question whether solutions develop singularities; the analysis and simulation of thermally-activated switching pathways; and development of more efficient and accurate numerical schemes.

Organizer: Robert V. Kohn
Courant Institute of Mathematical Sciences, New York University

4:30-4:50 Boundary Vortices for Thin Ferromagnetic Films
Roger Moser, New York University

4:55-5:15 Domain Wall Motion in Ferromagnetic Layers
Christoph Melcher, University of Minnesota

5:20-5:40 Schrödinger Maps and Landau-Lifshitz Equations
Helena McGahagan, New York University

5:45-6:05 Cross-Tie Walls in Soft Ferromagnetic Films
Antonio Desimone, Max Planck Institute, Germany

Sunday, May 23

MS14 (For Part II, see MS9)

Computational Modelling of Microstructural Evolution: Part III

4:30 PM-6:10 PM

Room: Regency Ballroom D

Microstructures have a key role in determining properties of materials. Thus, understanding their evolution during processing or operation is necessary in achieving desired material properties and optimized performance. The recent advances in numerical methods and computational power have provided a fertile ground for computational investigations to flourish in this traditionally experimental field, and models and simulations are becoming more and more accurate and robust. In this mini-symposium, we gather researchers utilizing various modelling methods. In particular, we bring together both view points from the sharp interface and diffuse interface methods, as well as those of experimental work.

Organizer: Katsuyo Thornton
Northwestern University

Organizer: Peter Voorhees
Northwestern University

4:30-4:50 Dynamics of Precipitates in Three-dimensional Elastic Media
Qing Nie, University of California, Irvine

4:55-5:15 The Effect of Inhomogeneity on Microstructure Evolution
Xiaofan Li, Illinois Institute of Technology; Qing Nie, University of California, Irvine; and Katsuyo Thornton and Peter Voorhees, Northwestern University

5:20-5:40 Controlling the Shape of Growing 3D Crystals and Supression of the Mullins-Sekerka Instability
John Lowengrub, University of California, Irvine

5:45-6:05 Modeling Effects of Stress on the Evolution of Polycrystalline Microstructures
Isabela Vrinceanu and W. Craig Carter, Massachusetts Institute of Technology

Sunday, May 23

MS15 (For Part II, see MS10)

Superconductivity, Ginzburg-Landau Theory, and Related Topics: Part III

4:30 PM-6:10 PM

Room: Regency Ballroom E

With the recent award of the Nobel Prize in Physics, a renewed attention has been focused on theoretical foundations of superconductivity and superfluidity. The award recognizes Ginzburg-Landau theory as "being of great importance in physics ...". The speakers in this minisymposium will describe their recent research in Ginzburg-Landau theory and related phenomena including: (1) the development or refinement of mezoscale and macroscale models for quantized vortices; (2) mathematical aspects of the Ginzburg-Landau theory and applications in the practical study of dynamics of vortices in superconductivity, superfluidity, and in problems describing defects in liquid crystals; (3) numerical studies of the vortex phenomena.

Organizer: Qiang Du
Pennsylvania State University

Organizer: Leonid Berlyand
Pennsylvania State University

Organizer: Dmitry Golovaty
University of Akron

4:30-4:50 A Comparison of Models for SNS Junctions via Ginzburg-Landau Theory
Peter Sternberg and Jacob Rubinstein, Indiana University and Michelle Schatzman, Université; Claude Bernard Lyon 1, Villeurbanne, France

4:55-5:15 The Zero Set of the Order Parameter
Jacob Rubinstein, Indiana University

5:20-5:40 Phase Patterns of the Ginzburg-Landau Equation with Discontinuous Coefficients in a Ring
Yoshihisa Morita and Satoshi Kosugi, Ryukoku University, Japan

5:45-6:05 Ginzburg-Landau Equation in a Thin Domain
Shuichi Jimbo, Hokkaido University, Japan

Monday, May 24

Registration Open

8:00 AM-5:00 PM

Room: Regency Foyer

Internet Cafe

8:00 AM-5:00 PM

Room: Redondo B

Monday, May 24

IP4

Inverse Design Problems in Electromagnetic and Nano-Photonics

8:30 AM-9:15 AM

Room: Regency Ballroom A/B

Chair: Demetri Psaltis, California Institute of Technology

Photonic crystals, are 2 and 3 dimensional structures, that are the analog for electromagnetics of the semiconductor crystals that play such an important role in electronics. Thus Maxwell's equations are to photonic crystals, what Schrodinger's equation is to conventional crystals. Since photonic crystals are purely products of our imagination, the question has always been what is the exact structure that should be fabricated? Engineering design is formally a type of mathematical Inverse Problem. The design goal is a certain electromagnetic specification or desired electromagnetic performance. It is necessary to work backward from that goal to the exact design of the dielectric boundary that achieves the objective. For example, in mathematics, the Level Set Method has emerged as an excellent tool that can contribute to algorithms for the optimization of boundaries and edges. In the Photonic Crystal field, the era of purely intuitive design may be obsolete. We must now concentrate more on design software, rational design, and the numerical solution of inverse problems. There are a number of inverse algorithms, including genetic algorithms, the error-propagation method, and simulated annealing that can contribute to future progress in photonic crystal design. It is expected that the study of photonic crystals will more and more be study and development of rational inverse design algorithms and software.

Eli Yablonovitch
University of California, Los Angeles

Monday, May 24

IP5

Anomolous Light Phenomena with Photonic Crystals

9:15 AM-10:00 AM

Room: Regency Ballroom A/B

Chair: Demetri Psaltis, California Institute of Technology

Photonic crystals are periodic dielectric structures that have a band gap that forbids propagation of a certain frequency range of light. This and other properties of these systems enable one to control light with amazing facility and produce effects that are impossible with conventional optics. A quick introduction of the basic concepts involving these materials is presented followed by several examples where anomalous light behavior can be obtained. Examples include the possibility of negative refraction, sub-wavelength resolution, unusual Cerenkov radiation, bandwidth narrowing (without losses) and reverse Doppler shifts.

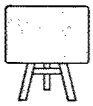
John D. Joannopoulos
Massachusetts Institute of Technology

Monday, May 24

PP1

Coffee Break and Poster Session I

10:00 AM-10:30 AM



Room: Regency Foyer & Manhattan Room

A System of A PDE Coupled with A Variational Inequality
Ming Fang, Norfolk State University and Robert Gilbert, University of Delaware

Atomistic and Continuum Models of Crystalline Solids
Weinan E and *Pingbing Ming*, Princeton University

A Biphasic Model for Local Cell-Matrix Mechanics in Articular Cartilage
Mansoor A. Haider, North Carolina State University

Development of a Micro-Macro Simulation Algorithm for Polymeric Fluids
Deepthika C. Senaratne and Kathleen Feigl, Michigan Technological University

Dynamics of the Morphological Evolution of Sputter Ripples
Ashwin Ramasubramaniam and Vivek Shenoy, Brown University

Comparison of Models for Frontal Polymerization
Stephen Cardarelli, *Dmitry Golovaty*, Laura Gross, Vitaliy Gyrya, and Jianping Zhu, University of Akron

Effect of Surface-Energy and Wetting Interaction Anisotropy on Self-Organization of Quantum Dots
Margo Levine and Alexander A. Golovin, Northwestern University

Disorder Effects in Photonic Crystal Structures
Walter R. Frei and Harley Johnson, University of Illinois, Urbana-Champaign

An Efficient Algorithm for Fracture Simulations
Phani K. Nukala and Srdan Simunovic, Oak Ridge National Laboratory

Coffee Break and Poster Session I, *continued*

A Discrete Model for the Elastic Field of a Surface Step
Cameron R. Connell, New Jersey Institute of Technology; Russel Caflisch and Erding Luo, University of California, Los Angeles; and Geoff Simms, HRL Laboratories, LLC

Algorithms for Classical Density Functional Theory
Andy Salinger, *Laura Frink*, and Mike A. Heroux, Sandia National Laboratories

Closure of the Set of Diffusion Functionals and That of Elasticity
Mohamed Camar-Eddine, University of Utah and P Seppecher, Universite de Toulon, France

Monday, May 24

MS16 (For Part V, see MS22)

Composites and Polycrystals: Part IV

10:30 AM-12:10 PM

Room: Regency Ballroom A

The emphasis of the minisymposium will be on effective properties of linear, as well as nonlinear, composites and polycrystals: rigorous homogenization techniques, bounds and estimates, exact relations between various effective physical properties, wave propagation, loss of ellipticity, discrete systems (lattices).

Organizer: Graeme W. Milton
University of Utah

Organizer: Pierre M. Suquet
CNRS, France

10:30-10:50 Can We Find the Structure of a Composite From its Effective Properties?
Elena Cherkaev, University of Utah

10:55-11:15 An Analytic Model of Composites with Locally Resonant Units
Ping Sheng, The Hong Kong University of Science and Technology, Hong Kong; Zhengyou Liu, Wuhan University, China; and C. T. Chan, Hong Kong University of Science and Technology, Hong Kong

11:20-11:40 Slowing Down the Light by a Photonic Crystal
Alexander Figotin and Ilya Vitebskiy, University of California, Irvine

11:45-12:05 Phononic Band Gap Structures and Localised Eigen-States
Alexander Movchan, University of Liverpool, United Kingdom

Monday, May 24

MS17 (For Part V, see MS23)

Multi-scale Modeling and Simulation of Complex Fluids: Part IV

10:30 AM-12:10 PM

Room: Regency Ballroom B

Complex fluids are materials exhibiting both fluid and non-fluid like behavior, which encompass solutions and melts of polymers, nanocomposites, liquid crystals, forms, emulsions, gels, and many biomaterials etc. Many fascinating and intriguing phenomena have been reported in flows of complex fluids, which are often related to effects of multiple spatial and time scales as well as the coupling between the macroscopic flow and materials' micro-structures. Modeling and simulation of complex fluids have been a challenge for the scientific community over the year.

Recently, the mathematics community has become more and more involved in research on these fascinating materials. The goal of the symposium at the meeting is to bring together researchers from different disciplines and different continents to exchange ideas and forge new collaborations to tackle issues in modeling and simulation of complex fluids.

Organizer: Chun Liu
Pennsylvania State University

Organizer: Qi Wang
Florida State University

Organizer: Pingwen Zhang
Peking University, China

Organizer: Claude Le Bris
ENPC/CERMICS, France

10:30-10:50 Well-Posedness and Simulation of Rod-like Models
Pingwen Zhang, Peking University, China

10:55-11:15 Numerical Methods for Multiscale Kinetic Problems
Shi Jin, University of Wisconsin, Madison

11:20-11:40 Epitaxial Growth without Slope Selection: Energetics, Coarsening, and Dynamic Scaling
Bo Li, University of Maryland

11:45-12:05 Coarse-graining and Adaptive Monte Carlo Simulation in Non-Equilibrium Lattice Systems
Markos A. Katsoulakis, University of Massachusetts, Amherst

Monday, May 24

MS18 (For Part III, see MS13)

Analytical and Numerical Aspects of Micromagnetics: Part IV

10:30 AM-12:10 PM

Room: Regency Ballroom C

The micromagnetic variational principle is a nonconvex variational problem whose local minima represent the stable magnetization patterns of a ferromagnetic body. The associated evolution, Landau-Lifshitz-Gilbert dynamics, describes magnetic switching and the response of a ferromagnet to a varying applied field. These models capture the remarkable multiscale complexity of magnetic materials. Their analysis and simulation raises fundamental and challenging issues of physics and mathematics. Current issues include: the identification of simpler reduced models in physically-relevant asymptotic regimes; the question whether solutions develop singularities; the analysis and simulation of thermally-activated switching pathways; and development of more efficient and accurate numerical schemes.

Organizer: Robert V. Kohn
Courant Institute of Mathematical Sciences, New York University

10:30-10:50 Magnetic Switching: pulsed astroids and thermal effects
Maria Reznikoff, New York University

10:55-11:15 Constructing Partially Regular Solutions for the Generalized Landau-Lifshitz-Gilbert Equations
Joy Ko, New York University

11:20-11:40 Another Thin-Film Limit of Micromagnetics
Valeriy Slastikov, Carnegie Mellon University and Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

11:45-12:05 Interaction Energies for Boundary Vortices in Thin Magnetic Films
Matthias Kurzke, Max Planck Institute, Germany

Monday, May 24

MS19

Conformal-mapping Methods for Microstructural Evolution

10:30 AM-12:10 PM

Room: Regency Ballroom D

For half a century, time-dependent conformal maps have been used to describe viscous fingering and related problems of continuous "Laplacian growth", where a free boundary moves in response to the gradient of a harmonic function (pressure, temperature, or concentration). In recent years, there has been an explosion of interest in extending such methods to more general models of microstructural evolution. A major advance in 1998 was the introduction of stochastic dynamics via the Hastings-Levitov method of iterated conformal maps for Diffusion-Limited Aggregation [Sander] (a few years before Stochastic Loewner Evolution). Other recent advances involve non-Laplacian conformally invariant transport processes [Bazant], as in continuous soldification from a flowing melt [Kornev] and stochastic Advection-Diffusion-Limited Aggregation [Bazant], and bi-harmonic free boundary problems, such as viscous sintering and brittle fracture [Crowdy].

Organizer: Martin Z. Bazant
Massachusetts Institute of Technology

10:30-10:50 Conformal Maps, Crossovers and Fixed Points in Diffusion-Limited
Leonard M. Sander, University of Michigan

10:55-11:15 Dynamics of Conformal Maps for a Class of Non-Laplacian Growth Phenomena
Martin Z. Bazant and Jaehyuk Choi, Massachusetts Institute of Technology; Benny Davidovitch, Harvard University; and Darren G. Crowdy, Imperial College of Science Technology and Medicine, United Kingdom

11:20-11:40 Growth of Cylindrical Filaments in Potential Flows
Konstantin G. Kornev, Princeton University

11:45-12:05 Conformal Mapping Methods in Viscous Sintering and Related Problems
Darren G. Crowdy, Imperial College of Science Technology and Medicine, United Kingdom

Monday, May 24

MS21 (For Part II, see MS27)

Accurate and Efficient Mathematical Methods for Analysis, Design, and Optimization of Photonic Crystal Structures: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom F

Photonic crystals have inspired a lot of interest recently due to their ability to control the propagation of electromagnetic waves. The photonic bandgap available in these periodic structures allow for designing the propagation path of optical beams by adding defects to the structure. Photonic crystal waveguides, cavities, bends, and couplers are among the devices that can be formed by adding defects to photonic crystals. Accurate and efficient mathematical modeling is essential for optimizing photonic crystal structures. The application of conventional methods for the numerical simulation of the electromagnetic problems to photonic crystals usually requires extensive memory and results in very long simulations. This mini-symposium is focused on the novel techniques for the efficient and accurate modeling of photonic crystal structures and the applications of these models to analysis, design, and optimization of photonic crystal devices. Both planar structures and photonic crystal fibers are covered in this minim-symposium.

Organizer: Ali Adibi
Georgia Institute of Technology

10:30-10:50 Theoretical and Experimental Analysis of Cylindrical Photonic Bandgap Transmission Fibers Across the Infrared Spectrum
Yoel Fink, Massachusetts Institute of Technology

10:55-11:15 Bandgap Confinement in Photonic Crystal Fibers, Bragg Fibers, and Bragg Onion Resonators
Yong Xu and Amnon Yariv, California Institute of Technology

11:20-11:40 A Spatial Fourier Transform Technique for the Analysis of General Photonic Crystal Waveguides
Aliakbar Jafarpour, Georgia Institute of Technology

11:45-12:05 Mathematical Tools for Quantum Optics of Photonic Crystals
Kazuaki Sakoda, National Institute for Materials Science

Monday, May 24

Lunch

12:10 PM-1:30 PM

Attendees on their own

IP6

Modeling the Mechanical Behavior of Granular Materials

1:30 PM-2:15 PM

Room: Regency Ballroom A/B

Chair: Richard James, University of Minnesota, Minneapolis

Granular materials are common in nature, in industry, and in the home. They are interesting because they exhibit behaviors characteristic of a solid or a fluid, depending upon the circumstances. They are important because natural hazards, such as slope failure and soil liquefaction, are threats to life and property and because granular materials are involved in many, if not most, industrial processes. Unfortunately, present theories for the prediction of deformations, failure, and flow of granular materials are far less reliable than those for classical solids and fluids. We will focus on the quasi-static, rate-independent behavior of granular materials and review recent theories for their deformation and failure. These involve incremental relations between stress and deformation that include a dependence on the state of the material. The goal is to identify the appropriate state variables from the consideration of force and moment equilibrium of the individual particles, to incorporate them through suitable averaging into the incremental stress-strain relation, and to describe their evolution with the deformation.

James Jenkins
Cornell University

Intermission

2:15 PM-2:30 PM

Monday, May 24

MS22 (For Part IV, see MS16)

Composites and Polycrystals: Part V

2:30 PM-4:10 PM

Room: Regency Ballroom A

The emphasis of the minisymposium will be on effective properties of linear, as well as nonlinear, composites and polycrystals : rigorous homogenization techniques, bounds and estimates, exact relations between various effective physical properties, wave propagation, loss of ellipticity, discrete systems (lattices).

Organizer: Graeme W. Milton
University of Utah

Organizer: Pierre M. Suquet
CNRS, France

2:30-2:50 Negative Hall coefficients: not the hole story
Graeme W. Milton, University of Utah

2:55-3:15 Multi-scale Stress Assessment in Composite Structures
Robert P. Lipton, Louisiana State University

3:20-3:40 Network Approximation for Effective Viscosity of Highly Concentrated Random Suspensions
Leonid Berlyand, Pennsylvania State University; Liliana Borcea, Rice University; and Alexander Panchenko, Washington State University

3:45-4:05 Elastically Optimal Microstructures in the High-porosity Regime
Blaise A. Bourdin, Louisiana State University and Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

Monday, May 24

MS23 (For Part IV, see MS17)

Multi-scale Modeling and Simulation of Complex Fluids: Part V

2:30 PM-4:10 PM

Room: Regency Ballroom B

Complex fluids are materials exhibiting both fluid and non-fluid like behavior, which encompass solutions and melts of polymers, nanocomposites, liquid crystals, forms, emulsions, gels, and many biomaterials etc. Many fascinating and intriguing phenomena have been reported in flows of complex fluids, which are often related to effects of multiple spatial and time scales as well as the coupling between the macroscopic flow and materials' micro-structures. Modeling and simulation of complex fluids have been a challenge for the scientific community over the year.

Recently, the mathematics community has become more and more involved in research on these fascinating materials. The goal of the symposium at the meeting is to bring together researchers from different disciplines and different continents to exchange ideas and forge new collaborations to tackle issues in modeling and simulation of complex fluids.

Organizer: Chun Liu
Pennsylvania State University

Organizer: Qi Wang
Florida State University

Organizer: Pingwen Zhang
Peking University, China

Organizer: Chun Le Bris
ENPC/CERMICS, France

2:30-2:50 Time-dependent Solutions to a PDE Model for Superconducting Materials
Patricia Bauman, Dan Phillips, and Hala Jadallah, Purdue University

2:55-3:15 Type I Superconductivity Near Critical Temperature
Xingbin Pan, National University of Singapore, Republic of Singapore

3:20-3:40 Flow Properties of Cholesteric Liquid Crystal Polymers
Zhenlu Cui, Florida State University

3:45-4:05 Title not available at time of publication
Peter Olmsted, University of Leeds, United Kingdom

Monday, May 24

MS24 (For Part II, see MS30)

Ferroelectrical Phenomena in Soft Materials: Part I

2:30 PM-4:10 PM

Room: Regency Ballroom C

Ferroelectric models are at the core of important research themes such as artificial muscles, robotics, video display, organic semiconductors, optical switching and telecommunications. Prototype ferroelectric models can be found in solid mechanics as well as in liquid crystals, polymeric systems, membranes, liquid crystal elastomers, gels and micelles.

Electron microscopy and experimental activity have provided a great deal of detailed information on structures. But the integration of mathematical modeling , analysis, and numerical simulation with experimental approaches promises to greatly increase our understanding.

The goal of this minisymposium is to bring together experts from materials science and mathematics, working on electrical properties of soft materials, to illuminate and explore the challenges that they present.

Organizer: Daniel Phillips
Purdue University

Organizer: Patricia Bauman
Purdue University

Organizer: Maria-Carme Calderer
University of Minnesota

2:30-2:50 Antiferroelectric and Ferroelectric Smectic Liquid Crystal Fibers of Bent-core Molecule
Antal Jakli, Kent State University; Daniel Kruerke, Technische Universitaet Berlin, Germany; and Geetha Nair, Centre for Liquid Crystal Research, Bangalore, India

2:55-3:15 Time Evolution of Nematic Liquid Crystals and Motion by Mean Curvature
M. Carme Calderer, University of Minnesota; *Dmitry Golovaty*, University of Akron; and Chun Liu, Pennsylvania State University

3:20-3:40 Cross-couplings Cut through Complexity: Banana Liquid Crystals
Patricia E. Cladis, Advanced Liquid Crystal Technologies, Inc.; Harald Pleiner, Max Planck Institute for Polymer Research, Germany; and Helmut Brand, Universitaet Bayreuth, Germany

3:45-4:05 Fast Switching of Electrically Driven Dual Frequency Liquid Crystals
Oleg Lavrentovich, Andrii Golovin, and Sergij Shiyanovskii, Kent State University

Monday, May 24

MS25 (For Part II, see MS31)

Modeling and Analysis of Grain Growths in Polycrystalline Materials: Part I

2:30 PM-4:10 PM

Room: Regency Ballroom D

The study of grain growths has a long history and yet still is an important area. In the case of polycrystalline materials, the grains -- their boundary structure, orientation, size and shape -- constitute the microstructures which in turn determine the overall material properties. Accurate understanding of their connections has profound implications in the manufacturing and design processes. This is particularly important due to the on-going need for the search of new materials. This mini-symposium will bring together different techniques of atomic and continuum modeling and analysis of grain growths. Comparison to experimental and numerical results will be emphasized.

Organizer: Alexander King
Purdue University

Organizer: Aaron Yip
Purdue University

2:30-2:50 Mesoscale Issues in Microstructure Simulation
Shlomo Ta'asan, Carnegie Mellon University

2:55-3:15 Atomic Force Microscopy Study of Grain Boundary Migration
Eugene Rabkin, Israel Institute of Technology, Israel and Y. Amouyal and L. Klinger, Tel Aviv University, Israel

3:20-3:40 Impurity Effects on Grain Boundary Migration: Theory and Computer Simulation
Mikhail I. Mendelev and David Srolovitz, Princeton University

3:45-4:05 Size Effects during Thermal Evolution of Bulk Nano-Crystalline Microstructures
Moneesh Upmanyu, Colorado School of Mines

Monday, May 24

MS26 (For Part II, see MS32)

Mathematical Modeling and Simulation of Granular Flows: Part I

2:30 PM-4:10 PM

Room: Regency Ballroom E

Granular flow is a major theme of the SIAM MS04 conference since it represents a frontier in the mathematical theory of condensed matter systems. By now, it is fairly well established that the kinetic theory of gases can be modified mainly by allowing for inelastic collisions to describe fast, dilute flows, but some basic open questions remain. For example, stretched tails of velocity distibutions in dilute, driven flows correspond to new non-equilibrium statistics. Perhaps even more fundamental issues arise in slow, dense flows, which seem to defy classical statistical mechanics and hydrodynamics, as long-lasting many-body contacts call for new mathematical approaches. These three symposia survey some recent developments in statistical and continuum theories for both dilute and dense flows in the context of experiments and molecular dynamics simulations.

Organizer: Martin Z. Bazant
Massachusetts Institute of Technology

Organizer: Irene Gamba
University of Texas

2:30-2:50 Shear Inelastic Diluted Flows Modeled by Boltzmann Equations
Irene Gamba, University of Texas

2:55-3:15 Continuum Simulations of Vertically Vibrated Granular Media
Jonathan L. Bougie, University of Texas, Austin; Sung Joon Moon, Princeton University; and Jack Swift and Harry Swinney, University of Texas, Austin

3:20-3:40 High-Energy Tails for Velocity Distributions in Rapid Granular Flows
Vladislav Panferov, University of Victoria, Canada

3:45-4:05 Lattice Dynamics and Noise Effects in Patterns in Oscillated Granular Layers
Harry Swinney, University of Texas, Austin

Monday, May 24

MS27 (For Part I, see MS21)

Accurate and Efficient Mathematical Methods for Analysis, Design, and Optimization of Photonic Crystal Structures: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom F

Photonic crystals have inspired a lot of interest recently due to their ability to control the propagation of electromagnetic waves. The photonic bandgap available in these periodic structures allow for designing the propagation path of optical beams by adding defects to the structure. Photonic crystal waveguides, cavities, bends, and couplers are among the devices that can be formed by adding defects to photonic crystals. Accurate and efficient mathematical modeling is essential for optimizing photonic crystal structures. The application of conventional methods for the numerical simulation of the electromagnetic problems to photonic crystals usually requires extensive memory and results in very long simulations. This mini symposium is focused on the novel techniques for the efficient and accurate modeling of photonic crystal structures and the applications of these models to analysis, design, and optimization of photonic crystal devices. Both planar structures and photonic crystal fibers are covered in this mini symposium.

Organizer: Ali Adibi
Georgia Institute of Technology

2:30-2:50 Homogenization of Wire Photonic Crystals Leading to Left-Handed Media
Didier Felbacq, GES UMR CNRS, France and Guy Bouchitte, Universite de Toulon et du Var, France

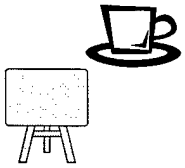
2:55-3:15 Scattering Matrix Techniques for Modelling Extended Photonic Crystal Devices
Lindsay C. Botten, Ara A Asatryan and Timothy N Langtry, University of Technology, Australia; Thomas P White, Ross C McPhedran, and C Martijn de Sterke, University of Sydney, Australia

3:20-3:40 Design of Novel Optical
Tanya Monro, University of Southampton, United Kingdom

3:45-4:05 Title not available at time of publication
Oskar Painter, California Institute of Technology

Tuesday, May 25

PP2



Coffee Break and Poster Session II

4:10 PM-4:30 PM

Room: Regency Foyer & Manhattan

Mathematical Analysis of a Simple 1D Discrete-Continuum Method for Materials Simulation
Frederic Legoll, CERMICS ENPC, France; Xavier Blanc, Universite Paris VI, France; and Claude Le Bris, CERMICS ENPC, France

Kinetics of Average N-hedra in 3-D Networks
Martin E. Glicksman, Rensselaer Polytechnic Institute

Mathematical Models of Aerogels
John A. Quintanilla, University of North Texas

Finite Element Simulations for the Burton-Cabrera-Frank Equations
Axel Voigt and Haußer Frank, Research Center Caesar, Germany

Estimating the Mechanical Properties of Amorphous Columnar Thin Films Using Md
Francesco Costanzo, *Gary L. Gray*, Pedro C. Andia, and Thomas J. Yurick, Pennsylvania State University

Fatigue Behaviour of Ferroelectrics
Santiago A. Serebrinsky, and Irene Arias and Michael Ortiz, California Institute of Technology

Equilibrium Shapes of Epitaxially Strained Islands with Finite Contact Angle
Oleg E. Shklyaev, Michael J. Miksis, and Peter W. Voorhees, Northwestern University

Identification of NiTi Alloy Thermal Expansion Coefficient Using Preisach Density Function.
William S. Galinaitis, Ferrum College

Mesh Optimization for the Quasicontinuum Method: A Generalization of Vale to Inelastic Problems
Jaime Marian, Jaroslaw Knap, and Michael Ortiz, California Institute of Technology

Full Two-Scale Expansion for Nonlinear Periodic Problems and Higher-Order Homogenized Problems
Valery Smyshlaev, University of Bath, United Kingdom and Kirill Cherednichenko, University of Oxford, United Kingdom

Effective Thermal Expansion of Multiphase Heterogeneous Medium
Vladimir Vinogradov, University of Utah

Monday, May 24

MS28

Homogenization in Discrete Systems

4:30 PM-6:10 PM

Room: Regency Ballroom A

Although in linear case the relation between continuum models and their discrete prototypes can be considered established, models with strong nonlinearity and nonconvex energy still present a considerable challenge. The corresponding discrete problems exhibit localization of deformation at the scale of the lattice, which makes continuum limit nontrivial. The overall ruggedness of the energy landscape leads to hysteresis and path dependence. In dynamics, the complexity of the micro-motion associated with multi- stability suggests that the homogenization must be necessarily thermodynamical. This mini-symposium addresses different aspects of this problem and presents some recent advances concerning the whole range of material behaviors from plasticity to fracture.

Organizer: Lev Truskinovsky
Ecole Polytechnique, France

Organizer: Andrea Braides
University of Rome, Italy

4:30-4:50 Atomistic and Continuum Models of Solids
Weinan E and Pingbing Ming, Princeton University

4:55-5:15 Coarse-Graining of Atomistic Binding Relations and Universal Macroscopic Cohesive Behavior
Michael Ortiz, California Institute of Technology

5:20-5:40 Mechanical Model of Latent Heating
Yalchin Efendiev, Texas A&M University and Lev Truskinovsky, Ecole Polytechnique, France

5:45-6:05 Surface Energies in Non-convex Discrete Systems
Marco Cicalese, Università di Napoli, Italy and Andrea Braides, University of Rome, Italy

Monday, May 24

MS29

Coarsening Dynamics and Morphology of Faceted Crystal Surfaces Far from Equilibrium

4:30 PM-6:10 PM

Room: Regency Ballroom B

This mini-symposium will consider the morphology and coarsening dynamics of crystaline surfaces driven by a bulk field (e.g., undercooled melt, deposition, elastic strain). The study of such non-equilibrium systems has received significant impetus from the discovery of nanoscale faceted pyramidal islands (quantum dots); objects of significant technological interest. The speakers will present both continuum and atomistic models which exhibit the dramatic effects that bulk/surface interaction has on crystal surface morphology, its coarsening dynamics and the associated scaling laws.

Organizer: Stephen J. Watson
Northwestern University

4:30-4:50 A Description of Strain-driven Formation of Semiconductor Nanostructures
Ben Freund, Brown University

4:55-5:15 The Evolution and Self Assembly of Quantum Dots on Surfaces
Peter Voorhees, Northwestern University

5:20-5:40 Scaling and Coarsening of Step Bunches
Joachim Krug, University of Cologne, Germany

5:45-6:05 Coarsening Dynamics of Faceted Crystal Surfaces
Stephen J. Watson, Northwestern University

Monday, May 24

MS30 (For Part I, see MS24)

Ferroelectrical Phenomena in Soft Materials: Part II

4:30 PM-6:10 PM

Room: Regency Ballroom C

Ferroelectric models are at the core of important research themes such as artificial muscles, robotics, video display, organic semiconductors, optical switching and telecommunications. Prototype ferroelectric models can be found in solid mechanics as well as in liquid crystals, polymeric systems, membranes, liquid crystal elastomers, gels and micelles.

Electron microscopy and experimental activity have provided a great deal of detailed information on structures. But the integration of mathematical modeling, analysis, and numerical simulation with experimental approaches promises to greatly increase our understanding.

The goal of this minisymposium is to bring together experts from materials science and mathematics, working on electrical properties of soft materials, to illuminate and explore the challenges that they present.

Organizer: Daniel Phillips
Purdue University

Organizer: Patricia Bauman
Purdue University

Organizer: Maria-Carme Calderer
University of Minnesota

4:30-4:50 Electro-mechanical Behavior of Ferroelectric Perovskites
Kaushik Bhattacharya, California Institute of Technology

4:55-5:15 The Phase Transition Between Chiral Nematic and Smectic C* Liquid Crystals
Sookyung Joo and Daniel Phillips, Purdue University

5:20-5:40 Mirrorless Lasing in Liquid Crystalline Bandgap Materials
Peter Palffy-Muhoray and Wenyi Cao, Kent State University; Antonio Munoz, Universidad Autonoma Metropolitana, Mexico; and Bahman Taheri, Kent State University

5:45-6:05 Cooperative Effects in a Dye/liquid Crystal System
David Kinderlehrer, Carnegie Mellon University

Monday, May 24

MS31 (For Part I, see MS25)

Modeling and Analysis of Grain Growths in Polycrystalline Materials: Part II

4:30 PM-6:10 PM

Room: Regency Ballroom D

The study of grain growths has a long history and yet still is an important area. In the case of polycrystalline materials, the grains -- their boundary structure, orientation, size and shape -- constitute the microstructures which in turn determine the overall material properties. Accurate understanding of their connections has profound implications in the manufacturing and design processes. This is particularly important due to the on-going need for the search of new materials. This mini-symposium will bring together different techniques of atomic and continuum modeling and analysis of grain growths. Comparison to experimental and numerical results will be emphasized.

Organizer: Alexander King
Purdue University

Organizer: Aaron Yip
Purdue University

4:30-4:50 Modelling Grain Growth in Crystalline Materials
John Cahn, National Institute of Standards and Technology and Jean Taylor, New York University

4:55-5:15 On Growth-Induced Rotation of Embedded Crystals
Jean Taylor, New York University and John Cahn, National Institute of Standards and Technology

5:20-5:40 Modeling of Grain Structure Evolution and Singular Diffusivity
Ryo Kobayashi, Hokkaido University, Japan

5:45-6:05 Phase-Field Modelling of Intergranular Films in Silicon Nitride
Catherine Bishop, Massachusetts Institute of Technology

Monday, May 24

MS32 (For Part III, see MS38)

Mathematical Modeling and Simulation of Granular Flows: Part II

4:30 PM-6:10 PM

Room: Regency Ballroom E

Granular flow is a major theme of the SIAM MS04 conference since it represents a frontier in the mathematical theory of condensed matter systems. By now, it is fairly well established that the kinetic theory of gases can be modified mainly by allowing for inelastic collisions to describe fast, dilute flows, but some basic open questions remain. For example, stretched tails of velocity distibutions in dilute, driven flows correspond to new non-equilibrium statistics. Perhaps even more fundamental issues arise in slow, dense flows, which seem to defy classical statistical mechanics and hydrodynamics, as long-lasting many-body contacts call for new mathematical approaches. These three symposia survey some recent developments in statistical and continuum theories for both dilute and dense flows in the context of experiments and molecular dynamics simulations.

Organizer: Martin Z. Bazant
Massachusetts Institute of Technology

Organizer: Irene Gamba
University of Texas

4:30-4:50 A Theory of Cooperative Diffusion in Dense Granular Flows
Martin Z. Bazant, Massachusetts Institute of Technology

4:55-5:15 Molecular Dynamics Simulations of Dense Granular Hopper Flows
James W. Landry, Sandia National Laboratories

5:20-5:40 Dense Granular Flows
Thomas C. Halsey, ExxonMobil Research

5:45-6:05 Order-parameter Description of Dense Granular Media
Igor Aranson, Argonne National Laboratory

Monday, May 24

MS33 (For Part II, see MS39)

Light and Wave Propagation in Inhomogeneous Media: Theory and Modeling: Part I

4:30 PM-6:10 PM

Room: Regency Ballroom F

In this minisymposium, we will study various wave phenomena in inhomogeneous media. with optical and photonic application. Wave interactions via resonant and evanscent modes and nonlinear properties of the material will be the focus of the minisymposium. Both mathematical theory (Session I) and modeling and optimization techniques (Session II) will be addressed.

Organizer: Alexander Figotin
University of California, Irvine

Organizer: Wei Cai
University of North Carolina, Charlotte

4:30-4:50 Nonlinear Maxwell Equations in Inhomogeneous Media
Alexander Figotin, University of California, Irvine

4:55-5:15 On Spectra of "Soft Wall" Waveguides
Peter Kuchment, Texas A&M University

5:20-5:40 Anomalous Transmission in the Presence of Guided Modes
Stephen P. Shipman, Louisiana State University

5:45-6:05 Resonances and Bound States in Periodic Slab Structures
Stephanos Venakides, Duke University

Tuesday, May 25

Registration Open
8:00 AM-5:00 PM
Room: Redondo Foyer

Internet Cafe
8:00 AM-5:00 PM
Room: Redondo B

IP7

Electron Transport and Dissipation in Nanoscale Devices

8:30 AM-9:15 AM

Room: Regency Ballroom A/B

Chair: Russel Caflisch, University of California, Los Angeles

We present a quantum-kinetic scheme for the calculation of non-equilibrium transport properties in nanoscale systems. Our approach is based on a Liouville-master equation for a reduced density operator and represents a fully quantum generalization of the well-known semi-classical Boltzmann kinetic equation. The approach allows us, in particular, to model transport situations under high applied fields by adopting periodic boundary conditions. Applications to nanoscale devices and molecular structures are discussed.

Roberto Car
Princeton University

Tuesday, May 25

IP8

Rare and Not-So-Rare Events in Material Science and Beyond

9:15 AM-10:00 AM

Room: Regency Ballroom A/B

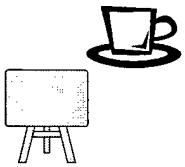
Chair: Russel Caflisch, University of California, Los Angeles

Many problems in material sciences but also physics, chemistry and biology can be abstractly formulated as a system that navigates over a complex energy landscape of high or infinite dimensions. Well-known examples include phase transitions of condensed matter, conformational changes of biopolymers, and chemical reactions. The energy landscape typically exhibits multiscale features, giving rise to the multiscale nature of the dynamics. The analysis of the transition pathways in such systems is a major challenges that we face in computational science. In this talk, I will review recent works done by scientists from several disciplines on probing such energy landscapes, and illustrate the techniques via examples like magnetic reversal micromagnetics, failure under stress in crystals structures, conformational change of peptides, etc.

Eric Vanden-Eijnden
Courant Institute of Mathematical Sciences, New York University

Tuesday, May 25

PP3



Coffee Break and Poster Session III

10:00 AM-10:30 AM

Room: Regency Foyer & Manhattan

Misfits in Two-Dimensional Laminated Polycrystals
Alexei Novikov, Pennsylvania State University

Multi-Scale Modeling and Electrokinetic Techniques in Sediment Acoustics
Gareth Block, University of Texas, Austin

Numerical Study of Transitions in Nematics
Arup Mukherjee, Montclair State University and Bagisa Mukherjee, Pennsylvania State University

On the Application of Thomas' and Poisson Branching Point Processes to Triboemission
Gustavo J. Molina, Georgia Southern University; A. Ritter and Michael Furey, Virginia Polytechnic Institute; and Czeslaw Kajdas, Warsaw University of Technology, Poland

On Multiscale Coupling in Polymer Fluids
Chun Liu, Pennsylvania State University

Motion of Contact Line of a Crystal Over the Edge of Solid Mask in Selective Area Epitaxy
Mikhail V. Khenner, State University of New York, Buffalo

Optimum Definition of Metal Tests Mechanical Properties (statistical Approach)
Arnold Korkhin, National Mining University

On a Class of Young Measures Arising in the Nonlinear Membrane Theory
Marian Bocea and Irene Fonseca, Carnegie Mellon University

Modeling Wetting and Spreading in Reactive Systems
Bruce T. Murray and Quan Yang, State University of New York, Binghamton

Nano-Composite Material Properties: Homogenization over Flow-Induced Orientational Distributions
Greg Forest, University of North Carolina, Chapel Hill; Xiaoyu Zheng, University of North Carolina; Robert P. Lipton, Louisiana State University; Ruhai Zhou, University of North Carolina; and Qi Wang, Florida State University

Nonlinear Isotropic Composites ?
Gal Debotton and Ilia Hariton, Ben-Gurion University of the Negev, Isreal

Tuesday, May 25

MS34 (For Part II, see MS40)

Contemporary Calculus of Variations for Advanced Materials: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom A

New advances in the mathematical sciences are required to provide the appropriate setting for the study and even the formulation of questions related to materials stability and instability. The goal of this minisymposium is to explore current progress and to stimulate the development of computational and variational techniques in partial differential equations and systems, as these contribute to a better understanding of microstructures, thin structures, phase transformations, magnetic materials, materials design, and other physical questions.

Organizer: Shlomo Ta'asan
Carnegie Mellon University

Organizer: Irene Fonseca
Carnegie Mellon University

Organizer: David Kinderlehrer
Carnegie Mellon University

Organizer: Giovanni Leoni
Carnegie Mellon University

10:30-10:50 A Random Weak Membrane Model
Andrea Braides, University of Rome, Italy

10:55-11:15 Regularity Results for Nonconvex Variational Problems
Georg K. Dolzmann, University of Maryland, College Park

11:20-11:40 Nematic Elatomers: A Case Study on Quasiconvex Envelopes Coming from Materials Science
Antonio De Simone, SISSA

11:45-12:05 Single-slip Elastoplastic Microstructures
Florian Thiel, University of Warwick, United Kingdom

Tuesday, May 25

MS35 (For Part II, see MS41)

Multiscale and Stochastic Modeling Methods: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom B

This minisymposium will review the current status and the challenges that remain in the exciting area of multiscale methods and stochastic methods.

Organizer: Weinan E
Princeton University

Organizer: Michael Ortiz
California Institute of Technology

Organizer: Emily Carter
University of California, Los Angeles

Organizer: Eric Vanden-Eijnden
Courant Institute of Mathematical Sciences, New York University

10:30-10:50 Modeling Iron at the bcc—hcp Phase Boundary
Kyle J. Caspersen, University of California, Los Angeles; Adrian Lew, Stanford University; Michael Ortiz, California Institute of Technology; Emily Carter, University of California, Los Angeles

10:55-11:15 Coarsening in stochastically perturbed Ginzburg-Landau gradient flows
Ibrahim Fatkullin, California Institute of Technology; Eric Vanden-Eijnden, Courant Institute of Mathematical Sciences, New York University

11:20-11:40 A Multiscale Method for the Dynamics of Solids at Finite Temperature
Xiantao Li, Princeton University

11:45-12:05 Martensitic Transition Pathways of Metallic Materials
Di Liu, Courant Institute of Mathematical Sciences, New York University

Tuesday, May 25

MS36 (For Part II, see MS42)

Active Materials: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom C

The minisymposium active materials will have presentations in electro-active polymers, ferroelectrics, shape memory alloys, and and ferromagnetic shape memory alloys, covering both mathematical and physical aspects of active materials of current interests.

Organizer: Jiangyu Li
University of Nebraska, Lincoln

10:30-10:50 Magnetic Tiles - A New Perspective on Ferromagnetic Shape Memory Alloys
Harsh Chopra, State University of New York, Buffalo

10:55-11:15 Modeling Magnetic-field-induced Strain in Ni-Mn-Ga
Miguel Marioni, Massachusetts Institute of Technology

11:20-11:40 Ferromagnetic Shape Memory Composites
Liping Liu, University of Minnesota

11:45-12:05 Magnetization Reversal and Hysteresis in Nanocrystalline Ferromagnets
Jiangyu Li, University of Nebraska, Lincoln

Tuesday, May 25

MS37 (For Part II, see MS43)

Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom D

Domain coarsening and coagulation processes arise in many areas of materials science, such as epitaxial growth, aging of metal alloys or in the evolution of granular materials. The speakers will discuss recent developments in experiment, modeling and analysis of these phenomena. A particular focus of this minisymposium will be on dynamic scaling, that is on the question whether a process displays universal scaling laws or whether transient behavior that reflects the influence of initial data is most relevant.

Organizer: Robert L. Pego
University of Maryland, College Park

Organizer: Barbara Niethammer
Humboldt University at Berlin, Germany

10:30-10:50 On the Effect of Screening and Correlation in Domain Coarsening
Barbara Niethammer, Humboldt University at Berlin, Germany; Felix Otto, University of Bonn, Germany; and Andreas Hoenig, Universitaet Bonn, Germany

10:55-11:15 Long-time Asymptotics of the LSW Model
Juan Velazquez, Universidad Complutense de Madrid, Spain

11:20-11:40 Coarsening Processes in Homoepitaxial Thin Films: Atomistic and Continuum Modeling
James Evans and Da-Jiang Liu, Iowa State University; Conrad Stoldt, University of Colorado; and Patricia Thiel, Iowa State University

11:45-12:05 Upper Bounds on Coarsening Rates for an Epitaxial Growth Model
Xiaodong Yan, Michigan State University and Robert V. Kohn, New York University

Tuesday, May 25

MS38 (For Part II, see MS32)

Mathematical Modeling and Simulation of Granular Flows: Part III

10:30 AM-12:10 PM

Room: Regency Ballroom E

Granular flow is a major theme of the SIAM MS04 conference since it represents a frontier in the mathematical theory of condensed matter systems. By now, it is fairly well established that the kinetic theory of gases can be modified mainly by allowing for inelastic collisions to describe fast, dilute flows, but some basic open questions remain. For example, stretched tails of velocity distibutions in dilute, driven flows correspond to new non-equilibrium statistics. Perhaps even more fundamental issues arise in slow, dense flows, which seem to defy classical statistical mechanics and hydrodynamics, as long-lasting many-body contacts call for new mathematical approaches. These three symposia survey some recent developments in statistical and continuum theories for both dilute and dense flows in the context of experiments and molecular dynamics simulations.

Organizer: Martin Z. Bazant
Massachusetts Institute of Technology

Organizer: Irene Gamba
University of Texas

10:30-10:50 Effective Temperature in Dense Granular Systems
Herman Makse, Levich Institute

10:55-11:15 Two-dimensional Equilibria Related to Steady Granular Flow in a Conical Hopper
Michael Shearer, North Carolina State University

11:20-11:40 Equation-Free Coarse-Grained Analysis of Granular Flows
Sung Joon Moon, Sankaran Sundaresan, and Ioannis Kevrekidis, Princeton University

11:45-12:05 The Mystery of Booming Sand Dunes
Melany Hunt, California Institute of Technology

Tuesday, May 25

MS39 (For Part I, see MS33)

Light and Wave Propagation in Inhomogeneous Media: Theory and Modeling: Part II

10:30 AM-12:10 PM

Room: Regency Ballroom F

In this minisymposium, we will study various wave phenomena in inhomogeneous media. with optical and photonic application. Wave interactions via resonant and evanscent modes and nonlinear properties of the material will be the focus of the minisymposium. Both mathematical theory (Session I) and modeling and optimization techniques (Session II) will be addressed.

Organizer: Alexander Figotin
University of California, Irvine

Organizer: Wei Cai
University of North Carolina, Charlotte

10:30-10:50 Photonic Waveguide of Coupled Microcavities with Whispering Gallery Modes
Wei Cai, University of North Carolina, Charlotte

10:55-11:15 Optimal Design of Photonic Crystals
David Dobson, University of Utah

11:20-11:40 High-order Fourier/ Chebyshev Methods for Large Eigenvalue Problems of Photonics
Leonid A. Kunyansky, University of Arizona

11:45-12:05 A New Boundary Integral Equation method for Photonic Crystal Devices
Hongwei Cheng, Madman Optics

Lunch

12:30 PM-1:30 PM

Attendees on their own

Tuesday, May 25

IP9

Accelerated Molecular Dynamics Methods

1:30 PM-2:15 PM

Room: Regency Ballroom A/B

Chair: Robert Phillips, California Institute of Technology

A significant problem in the atomistic simulation of materials is that molecular dynamics simulations are limited to nanoseconds, while important reactions and diffusive events often occur on time scales of microseconds and longer. Although rate constants for slow events can be computed directly using transition state theory (with dynamical corrections, if desired, to give exact rates), this requires first knowing the transition state. Often, however, we cannot even guess what events will occur. For example, in vapor-deposited metallic surface growth, surprisingly complicated exchange events are pervasive. I will discuss recently developed methods (hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics) for treating this problem of complex, infrequent-event processes. Building on statistical mechanical principles, these methods are designed to directly accelerate the dynamics to achieve longer times without prior knowledge of the available reaction paths. I will present our latest method developments and some recent applications, including metallic surface growth, deformation and dynamics of carbon nanotubes, and annealing after radiation damage events in MgO.

Arthur Voter
Los Alamos National Laboratory

Intermission

2:15 PM-2:30 PM

Tuesday, May 25

MS40 (For Part III, see MS46)

Contemporary Calculus of Variations for Advanced Materials: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom A

New advances in the mathematical sciences are required to provide the appropriate setting for the study and even the formulation of questions related to materials stability and instability. The goal of this minisymposium is to explore current progress and to stimulate the development of computational and variational techniques in partial differential equations and systems, as these contribute to a better understanding of microstructures, thin structures, phase transformations, magnetic materials, materials design, and other physical questions.

Organizer: Shlomo Ta'asan
Carnegie Mellon University

Organizer: Irene Fonseca
Carnegie Mellon University

Organizer: David Kinderlehrer
Carnegie Mellon University

Organizer: Giovanni Leoni
Carnegie Mellon University

2:30-2:50 Existence Results for Variational Models in Fracture Mechanics
Gianni Dal Maso, SISSA, Trieste, Italy

2:55-3:15 A Variational Formulation for the Dislocations on Crystals
Adriana Garroni, Universita di Roma "La Sapienza," Italy

3:20-3:40 Renormalized Energy and Forces on Dislocations
Giovanni Leoni, Carnegie Mellon University

3:45-4:05 Cross-Tie Patterns in Micromagnetics-Type Phase Transition Models
Sylvia Serfaty, Courant Institute of Mathematical Sciences, New York University

Tuesday, May 25

MS41 (For Part III, see MS47)

Multiscale and Stochastic Modeling Methods: Part II

2:30 PM-4:35 PM

Room: Regency Ballroom B

This minisymposium will review the current status and the challenges that remain in the exciting area of multiscale methods and stochastic methods.

Organizer: Weinan E
Princeton University

Organizer: Michael Ortiz
California Institute of Technology

Organizer: Emily Carter
University of California, Los Angeles

Organizer: Eric Vanden-Eijnden
Courant Institute of Mathematical Sciences, New York University

2:30-2:50 Nonlinear Elasticity of Carbon Nanotubes from Atomistic Models
Marino Arroyo, California Institute of Technology

2:55-3:15 Ttile not available at time of publication
Noam Berstein, Naval Research Laboratory

3:20-3:40 Mathematical and Numerical Analysis of Some Micro/macro Models for Solids
Claude Le Bris, CERMICS ENPC, France

3:45-4:05 Massively Parallel Dislocation Dynamics and Crystal Plasticity
Wei Cai, Vasily V. Bulatov, Tim G. Pierce, Masato Hiratani, Moono Rhee, and Meijie Tang, Lawrence Livermore National Laboratory

4:10-4:30 Ttile not available at time of publication
Jaime Marian, California Institute of Technology

Tuesday, May 25

MS42 (For Part I, see MS36)

Active Materials: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom C

The minisymposium active materials will have presentations in electro-active polymers, ferroelectrics, shape memory alloys, and and ferromagnetic shape memory alloys, covering both mathematical and physical aspects of active materials of current interests.

Organizer: Jiangyu Li
University of Nebraska, Lincoln

2:30-2:50 Experimentally-Based Mathematical Modeling of the Nano-Scale Mechanisms of Actuation of Ionic Polymer Metal Composites
Sia Nemat-Nasser, University of California, San Diego

2:55-3:15 High Dielectric Constant Polymer Composites - Effect of the Morphology and Physical Properties of the Constituents
Qiming Zhang, Pennsylvania State University

3:20-3:40 Formation and Motion of Phase Boundary in Nano-Grained Polycrystalline
Qingping Sun, The Hong Kong University of Science and Technology, Hong Kong

3:45-4:05 Energy-minimizing Microstructures in Multiphase Elastic Solids
Kaushik Bhattacharya, California Institute of Technology, *Isaac Chenchiah,* Max Planck Institute, Germany

Tuesday, May 25

MS43 (For Part III, see MS49)

Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part II

2:30 PM-4:10 PM

Room: Regency Ballroom D

Domain coarsening and coagulation processes arise in many areas of materials science, such as epitaxial growth, aging of metal alloys or in the evolution of granular materials. The speakers will discuss recent developments in experiment, modeling and analysis of these phenomena. A particular focus of this minisymposium will be on dynamic scaling, that is on the question whether a process displays universal scaling laws or whether transient behavior that reflects the influence of initial data is most relevant.

Organizer: Robert L. Pego
University of Maryland, College Park

Organizer: Barbara Niethammer
Humboldt University at Berlin, Germany

2:30-2:50 Coarsening of Fluid Films
Karl Glasner, University of Arizona and Tom Witelski, Duke University

2:55-3:15 Coarsening Dynamics in a Model of Shear Bands
Tom Witelski, Duke University

3:20-3:40 Evolution of Pattern Complexity in Cahn-Hilliard Models
Thomas Wanner, George Mason University; Marcio Gameiro, Georgia Institute of Technology; and Konstantin Mischaikow, Georgia Institute of Technology

3:45-4:05 Asymptotics and Coarsening in Grain Growth Models
Ibrahim Fatkullin, California Institute of Technology and Valeriy Slastikov, Carnegie Mellon University

Tuesday, May 25

MS44

Mathematical Modeling and Simulation of Granular Flows: Part IV

2:30 PM-4:10 PM

Room: Regency Ballroom E

Granular flow is a major theme of the SIAM MS04 conference since it represents a frontier in the mathematical theory of condensed matter systems. By now, it is fairly well established that the kinetic theory of gases can be modified mainly by allowing for inelastic collisions to describe fast, dilute flows, but some basic open questions remain.

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For example, the stretched tails of velocity distributions in dilute, driven flows correspond to new non-equilibrium statistics. Perhaps even more fundamental issues arise in slow, dense flows, which seem to defy classical statistical mechanics and hydrodynamics, as long-lasting many-body contacts call for new mathematical approaches. These three symposia survey some recent developments in statistical and continuum theories for both dilute and dense flows in the context of experiments and molecular dynamics simulations.

Organizer: Martin Z. Bazant
Massachusetts Institute of Technology

Organizer: Irene Gamba
University of Texas

4:45-6:40 The Inelastic Maxwell Model
Eli Ben-Naim, Los Alamos National Laboratory

Tuesday, May 25

MS45

Modes and Resonance in Periodic Structures

2:30 PM-4:10 PM

Room: Regency Ballroom F

[Proposed in coordination with the minisymposium on photonic devices and electromagnetic waves in complex media.]

Guided and quasi-guided modes are intimately related to extraordinary scattering characteristics in periodic structures. The phenomena hold promise for the design of integrated optics, lasers, and filters.

The complex interplay between modes and resonance in periodic structures is a new discovery, and the past few years have seen an effort to develop mathematical theories that explain the phenomena.

Presentations will address the mathematical theory of optical resonance with particular reference to small-scale defects, nonlinear multi-scale optics, nanoscale structures, micro-resonators, and plasmons.

Organizer: Stephen P. Shipman
Louisiana State University

2:30-2:50 Waveguide-plasmon Polaritons in Photonic Crystal Slabs with Metal Nanowires
Sergei Tikhodeev, Russian Academy of Sciences, Russia

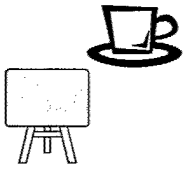
2:55-3:15 Transmission of Electromagnetic Waves through Single and Periodically Structured Subwavelength Apertures
Luis Martin-Moreno, University of Zaragoza, Spain

3:20-3:40 Complete Transmission Through a Two-Dimensional Diffraction Grating
Gregory Kriegsmann, New Jersey Institute of Technology

3:45-4:05 Effective Fields and Nonlinear Optical Propagation in Artificially Structured Materials
John Sipe, University of Toronto, Canada

Tuesday, May 25

PP4



Coffee Break and Poster Session IV

4:10 PM-4:30 PM

Room: Regency Foyer & Manhattan

The Effect of Tri-Junction Conditions in Droplet Solidification
Vladimir S. Ajaev, Southern Methodist University and Stephen H. Davis, Northwestern University

Oscillatory Pattern Formation in a Driven Binary Immiscible Fluid
Olga Kuksenok, David Jasnow, and Anna Balazs, University of Pittsburgh

Topological Complexity and the Dynamics of Coarsening
Igor Savin, Roberto Mendoza, Katsuyo Thornton, and Peter Voorhees, Northwestern University

Surface and Interface Effects in Solid Films
Tatiana Savin, Peter Voorhees, and Stephen H. Davis, Northwestern University

Surface-Directed Spinodal Decomposition in a Stressed Thin Film
Steven M. Wise and Jun-Seok Kim, University of California, Irvine and William Johnson, University of Virginia

Regularized Anisotropic Mean Curvature Flow of Curves
Axel Voigt and Haußer Frank, Research Center Caesar, Germany

Universality of Scaling in Fracture
Phani K. Nukala and Srdan Simunovic, Oak Ridge National Laboratory

Phase-Field Approximations for Step-Flow Models
Axel Voigt and Andreas Rätz, Research Center Caesar, Germany

The Role of Shear in the Onset of the Bcc to Hcp Stress-Induced Martensitic Transformation in Iron
Adrian Lew, Stanford University; Kyle J. Caspersen, University of California, Los Angeles; Michael Ortiz, California Institute of Technology; and Emily Carter, University of California, Los Angeles

State-of-the-Art Optimization Techniques for Electronic Structure Calculations
Marielba Rojas, Yonas Abraham, Natalie Holzwarth, and Robert Plemmons, Wake Forest University

Solitary Waves in Layered Nonlinear Media
Darryl Yong, Harvey Mudd College and Randy LeVeque, Washington University

Time Reversal Numerical Simulations for Randomly Layered Media
Mansoor A. Haider, North Carolina State University; Kurang Mehta, Colorado School of Mines; and Jean-Pierre Fouque, North Carolina State University

Simulation of Coarsening Faceted Crystal Surfaces: Dynamic Scalings, Correlations and Surface Statistics.
Scott Norris and Stephen J. Watson, Northwestern University

Global Feedback Control of a Long-Wave Morphological Instability
Alexander A. Golovin, Northwestern University; Alexander Nepomnyashchy, Technion - Israel Institute of Technology, Israel; Valery Gubareva, Technion Israel Institute of Technology, Israel; Vadim Panfilov, University of Nevada, Reno

Tuesday, May 25

MS46 (For Part II, see MS40)

Contemporary Calculus of Variations for Advanced Materials: Part III

4:30 PM-6:10 PM

Room: Regency Ballroom A

New advances in the mathematical sciences are required to provide the appropriate setting for the study and even the formulation of questions related to materials stability and instability. The goal of this minisymposium is to explore current progress and to stimulate the development of computational and variational techniques in partial differential equations and systems, as these contribute to a better understanding of microstructures, thin structures, phase transformations, magnetic materials, materials design, and other physical questions.

Organizer: Shlomo Ta'asan
Carnegie Mellon University

Organizer: Irene Fonseca
Carnegie Mellon University

Organizer: David Kinderlehrer
Carnegie Mellon University

Organizer: Giovanni Leoni
Carnegie Mellon University

4:30-4:50 Can Triple Junction Energy Contribute to the Driving Force for Grain Growth?
Alex King, Purdue University

4:55-5:15 A Reduced Model for Two-dimensional Grain Growth
Barbara Niethammer, Humboldt University at Berlin, Germany

5:20-5:40 Abnormal Grain Growth and the Potts Model
A. D. Rollett, Carnegie Mellon University

5:45-6:05 Boundary Tracking Simulation of Anisotropic Grain Growth and Grain Boundary Statistics
Peng Yu, Pennsylvania State University

Tuesday, May 25

MS47 (For Part II, see MS41)

Multiscale and Stochastic Modeling Methods: Part III

4:30 PM-6:35 PM

Room: Regency Ballroom B

This minisymposium will review the current status and the challenges that remain in the exciting area of multiscale methods and stochastic methods.

Organizer: Weinan E
Princeton University

Organizer: Michael Ortiz
California Institute of Technology

Organizer: Emily Carter
University of California, Los Angeles

Organizer: Eric Vanden-Eijnden
Courant Institute of Mathematical Sciences, New York University

4:30-4:50 Mixed Continuum/ atomistic Analysis of Nanovoid Cavitation
Michael Ortiz, California Institute of Technology and Jaroslaw Knap, California Institute of Technology

4:55-5:15 Title not available at time of publication
Robert E. Rudd, Lawrence Livermore National Laboratory

5:20-5:40 Coupling Kinetic Monte-Carlo and Continuum Models
Tim Schulze, University of Tennessee

5:45-6:05 Title not available at time of publication
Eric Vanden-Eijnden, New York University

6:10-6:30 Thermal Fluctuations on Large Domains
Maria Reznikoff, New York University

Tuesday, May 25

MS48

Lattice Models for Materials: Mathematical Results and Open Problems

4:30 PM-6:10 PM

Room: Regency Ballroom C

Key topics of the minisymposium are differential-difference equations arising from - atomistic models in solid mechanics - diffusion and transport on lattices - deposition kinetics and growth and their relationship with continuum limits in suitable asymptotic regimes.

Organizer: Florian Theil
University of Warwick, United Kingdom

4:30-4:50 Crystallization in two dimensions
Florian Theil, University of Warwick, United Kingdom

4:55-5:15 Elastic Crystals at Nonzero Temperature in Terms of Gibbs States
Roman Kotecky, Charles University, Czech Republic

5:20-5:40 Langevin Equations for Driven Lattice Systems
Dimitri D. Vvedensky, Imperial College London, United Kingdom

5:45-6:05 Discrete Traveling Waves: Defects in Crystals
Ana Carpro, Universidad Complutenic de Madrid, Spain

Tuesday, May 25

MS49 (For Part IV, see MS54)

Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part III

4:30 PM-6:10 PM

Room: Regency Ballroom D

Domain coarsening and coagulation processes arise in many areas of materials science, such as epitaxial growth, aging of metal alloys or in the evolution of granular materials. The speakers will discuss recent developments in experiment, modeling and analysis of these phenomena. A particular focus of this minisymposium will be on dynamic scaling, that is on the question whether a process displays universal scaling laws or whether transient behavior that reflects the influence of initial data is most relevant.

Organizer: Robert L. Pego
University of Maryland, College Park

Organizer: Barbara Niethammer
Humboldt University at Berlin, Germany

4:30-4:50 Dynamic Scaling in Smoluchowski's Coagulation Equation
Robert L. Pego, University of Maryland, College Park and Govind Menon, University of Wisconsin, Madison

4:55-5:15 Dynamic Scaling and Chaos in Burgers Turbulence
Govind Menon, University of Wisconsin, Madison and Robert L. Pego, University of Maryland, College Park

5:20-5:40 Self-similarity in Aggregation Problems with Continuous Input
Jonathan Wattis, University of Nottingham, United Kingdom

5:45-6:05 Mesoscopic Simulation for Surface Processes
David J. Horntrop, New Jersey Institute of Technology; Markos Katsoulakis, University of Massachusetts; and Dionisios Vlachos, University of Delaware

Tuesday, May 25

MS50

Long-range Interactions and Microstructure

4:30 PM-6:10 PM

Room: Regency Ballroom E

Repulsive long-range interactions often frustrate phase separation in systems undergoing first order phase transitions, leading to the formation of microstructures with complicated morphologies. The effect of these interactions is important in a variety of materials. Long-range forces may have different physical origins: they can come from fundamental electrostatic or magnetostatic interactions, or have an entropic origin resulting from the conformational changes of polymer chains, for example. This minisymposium will address the issues of the energetics in systems with competing short-range attractive and long-range repulsive interactions, with an emphasis on sharp interface limits, interfacial pattern morphologies, defects and nucleation.

Organizer: Xiaofeng Ren
Utah State University

Organizer: Cyrill B. Muratov
New Jersey Institute of Technology

4:30-4:50 Interfacial Patterns in Systems with Long-range Interactions of Coulomb type
Cyrill B. Muratov, New Jersey Institute of Technology

4:55-5:15 Nucleation in Fitzhugh-Nagumo System and Diblock Copolymer System
Juncheng Wei, Chinese University of Hong Kong, Hong Kong and Xiaofeng Ren, Utah State University

5:20-5:40 Phase Separartion in Diblock Copolymer Melts
Rustum Choksi, Simon Fraser University

5:45-6:05 Double Gyroid Morphology of the Diblock Copolymer Problem
Yasumasa Nishiura, Hokkaido University, Japan and Takashi Teramoto, Hokkaido University, Japan

Wednesday, May 26

Registration Open

8:00 AM-5:00 PM

Room: Regency Foyer

Internet Cafe

8:00 AM-5:00 PM

Room: Redondo B

Wednesday, May 26

IP10

Non-Slip vs. Slip: The Hydrodynamic Boundary Condition and the Moving Contact Line

8:30 AM-9:15 AM

Room: Regency Ballroom A/B

Chair: Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

Immiscible two-phase flow in the vicinity of the contact line (CL), where the fluid-fluid interface intersects the solid wall, is a classical problem that falls beyond the framework of conventional hydrodynamics. In particular, molecular dynamics (MD) studies have shown clear violation of the no-slip boundary condition. Numerous ad hoc models were proposed to resolve this incompatibility, but none can give realistic predictions in agreement with MD simulations. Consequently, a breakdown in the hydrodynamic description for the molecular-scale CL region has been suggested. We have uncovered the boundary condition governing the moving contact line, denoted the generalized Navier boundary condition (GNBC), and used this discovery to formulate a continuum hydrodynamics whose predictions are in remarkable quantitative agreement with the MD simulation results at the molecular level.

Ping Sheng
The Hong Kong University of Science and Technology, Hong Kong

Wednesday, May 26

IP11

Liquids, Solids and Elastic Heresy in Between—Is There a 2½ th State of Matter?

9:15 AM-10:00 AM

Room: Regency Ballroom A/B

Chair: Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

Several materials seem to be elastic intermediates. Rubber extends by as much as 1000\%, has a shear modulus 10^4 times smaller than its bulk modulus, and has liquid-like molecular mobility. Liquid crystals have orientational long-range order and thus (Frank) elasticity, but flow like liquids.

The elastic classification of matter is simple and strict. Solids require energy to change their shape, liquids do not-body rotations are elastically irrelevant. Thus rubber is really a solid, and liquid crystals are really liquids.

I discuss (with demonstrations) new materials breaking these apparently so simple and inflexible rules. I explore the consequences of such new elasticity and how it is manifested in practice.

Mark Warner
Cambridge University, United Kingdom

Coffee Break

10:00 AM-10:30 AM

Room: Regency Foyer

Wednesday, May 26

MS51 (For Part II, see MS57)

Quantitative Modeling in Biology: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom A

The advent of single molecule techniques has opened up the possibility of a new generation of mathematical modeling in the biological sciences. The aim of this symposium is to provide examples of the types of experiments being done in this field and of the mathematical models being put forth to greet them. Some of the particular examples to be included are: mechanics of DNA, physics of molecular motors, mechanics of biological membranes, cell motility and biological networks.

Organizer: Robert Phillips
California Institute of Technology

10:30-10:50 DNA Flexibility
Jon Widom, Northwestern University

10:55-11:15 Viruses as Physical Objects
Bill Gelbart, University of California, Los Angeles

11:20-11:40 Continuum Mechinics Models of DNA Minicircle Cyclization
John Maddocks, EPFL, France

Wednesday, May 26

MS52

Electronic Structure and Atomistic Simulations

10:30 AM-12:10 PM

Room: Regency Ballroom B

Forthcoming

Organizer: Michael Finnis
Queen's University, Belfast

10:30-10:50 Direct Generation of Wannier-like Functions (NMTO Minimal Basis Sets) from Multiple Scattering Theory and Applications
Ole K. Andersen, Max Planck Institute, Germany

10:55-11:15 Predicting the Optical and Structural Properties of Matter at the Nanoscale
James R. Chelikowsky, University of Minnesota

11:20-11:40 Calculation of Free Energy Surfaces in Classical and ab initio Molecular Dynamics
Michele Parrinello, ETH Zürich, Switzerland

11:45-12:05 Bond-order Potentials: Bridging the Electronic to Atomistic Modelling Hierarchies
David G. Pettifor, and *Ralf Drautz*, University of Oxford, United Kingdom

Wednesday, May 26

MS53 (For Part II, see MS59)

Challenges in Systems with Nematic and Smectic Order I

10:30 AM-12:10 PM

Room: Regency Ballroom C

Liquid crystals and their fascinating properties have been studied extensively since the 1920s, in particular in the physics and engineering literature. The most successful mathematical approach to the subject is the Ericksen-Leslie theory for nematic liquid crystals proposed in the 60s. Recent progress in the analysis of smectic liquid crystals was based on elasticity models within the framework of the Landau-De Gennes energy.

In the late 1990s, a completely new class of materials - so-called liquid crystal elastomers - was synthesised by cross-linking liquid crystal systems close to their transition temperature from the isotropic to the nematic or smectic phase. The key-feature of these new materials is the coupling of an orientational degree of freedom and the elasticity of the underlying network that is formed in the cross-linking process. The first mathematical theories for a class of nematic elastomers emerged in the past few years and have already substantially contributed to the understanding of the novel properties of these fascinating systems.

The goal of this minisymposium is to bring together experts in both fields in order to stimulate the exchange of ideas for the successful modeling, analysis, and numerical simulation of these materials.

Organizer: Chun Liu
Pennsylvania State University

Organizer: Georg K. Dolzmann
University of Maryland, College Park

Organizer: Antonio DeSimone
SISSA/Trieste, Italy

10:30-10:50 The Elasticity and Applications of Photoelastomers
Mark Warner, Cambridge University, United Kingdom

10:55-11:15 Nonlinear Elasticity of Liquid Crystal Gels and Applications to Cell Motility
Maria Carme Calderer and Hans Weinberger, University of Minnesota, Minneapolis

11:20-11:40 The Optomechanical Response of Nematic Elastomers
Peter Palffy-Muhoray and Tibor Toth-Katona, Kent State University; Miguel Camacho-Lopez, University of St. Andrews, United Kingdom; Heino Finkelmann, Albert-Ludwigs University; Luis Malacarne, University of Maringa, Brazil ; Michael J. Shelley, Courant Institute of Mathematical Sciences, New York University

11:45-12:05 Disclinations in Nematics Liquid Crystals
Paolo Biscari, Politecnico di Milano, Italy and Tim Sluckin, University of Southampton, United Kingdom

Wednesday, May 26

MS54 (For Part III, see MS49)

Dynamic Scaling and Models of Domain Coarsening and Coagulation: Part IV

10:30 AM-12:10 PM

Room: Regency Ballroom D

Domain coarsening and coagulation processes arise in many areas of materials science, such as epitaxial growth, aging of metal alloys or in the evolution of granular materials. The speakers will discuss recent developments in experiment, modeling and analysis of these phenomena. A particular focus of this minisymposium will be on dynamic scaling, that is on the question whether a process displays universal scaling laws or whether transient behavior that reflects the influence of initial data is most relevant.

Organizer: Robert L. Pego
University of Maryland, College Park

Organizer: Barbara Niethammer
Humboldt University at Berlin, Germany

10:30-10:50 Coarsening in Topologically Complex Systems: Experiments and Simulations
Peter Voorhees, Northwestern University

10:55-11:15 Gelation in Coagulation and Fragmentation Models
Miguel Escobedo, Universidad del País Vasco, Spain

11:20-11:40 Remarks on the LSW Theory of Coarsening
Nick Alikakos, University of Athens, Greece

11:45-12:05 Continuum Description of Profile Scaling in Nanostructure Decay
Dionisios Margetis, Massachusetts Institute of Technology and Michael Aziz and Howard Stone, Harvard University

Wednesday, May 26

MS55 (For Part II, see MS61)

Crack Propagation in Elastic and Viscoelastic Solids: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom E

The minisymposium addresses the analytical and experimental studies of subsonic and transonic crack propagation in elastic and viscoelastic bodies. Evidence of shear crack propagation in excess of the shear wave speed has been provided from observations of shallow crustal earthquakes and confirmed by recent experiments. The study of this phenomenon requires the design of new fracture criteria, finding fundamental solutions to the associated fracture problems, and developing new methods for matrix Wiener-Hopf factorization. Recent results in this area including the analysis of out-of plane corrugation waves and new experimental data on sub-Rayleigh and supershear rupture will be reported.

Organizer: Yuri A. Antipov
Louisiana State University

10:30-10:50 Vector Riemann-Hilbert Problem Associated with Crack Propagation in a Viscoelastic Medium
Yuri A. Antipov, Louisiana State University

10:55-11:15 Intersonic Crack Propagation along a Weak Plane in Solids
Yonggang Huang, University of Illinois, Urbana-Champaign

11:20-11:40 Laboratory Earthquakes
Ares J. Rosakis, California Institute of Technology

11:45-12:05 Corrugation Waves?
John Willis, University of Cambridge, United Kingdom

Wednesday, May 26

MS56 (For Part II, see MS62)

Mathematical Modeling of Electrochemical Systems: Part I

10:30 AM-12:10 PM

Room: Regency Ballroom F

Many modern materials processing techniques are based on electrochemical processes. This minisymposium is devoted to mathematical models, methods and approaches used for investigation of electrochemical processes relevant to materials science, especially to nanotechnology. The speakers will present recent results on mathematical modeling of such phenomena as anodic dissolution, electrodeposition, electroconvection, electrocapillary and electrokinetic effects, electrophoresis, effect of electric current on crystal growth, etc.

Organizer: Alexander A. Golovin
Northwestern University

10:30-10:50 Phase-Field Model of Electrochemistry
Geoffrey McFadden, William Boettinger, Jonathan Guyer, and James Warren, National Institute of Standards and Technology

10:55-11:15 The Effects of Applied Current on Growth Forms of Crystals
Lucien Brush, University of Washington

11:20-11:40 Models for Additive Effects on Microstructure and Surface Morphology During Electrodeposition
Mikko Haataja, McMaster University, Canada; David Srolovitz, Princeton University; and Corbett Battaile, Sandia National Laboratories

11:45-12:05 Formation of Regular Nano-Porous Structures During Anodization of Aluminum
Gogi Singh, Northwestern University; Igor Aronson, Argonne National Laboratory; and Alexander A. Golovin, Northwestern University

Lunch

12:30 PM-1:30 PM

Attendees on their own

Wednesday, May 26

MS57 (For Part III, see MS63)

Quantitative Modeling in Biology: Part II

1:30 PM-3:10 PM

Room: Regency Ballroom A

The advent of single molecule techniques has opened up the possibility of a new generation of mathematical modeling in the biological sciences. The aim of this symposium is to provide examples of the types of experiments being done in this field and of the mathematical models being put forth to greet them. Some of the particular examples to be included are: mechanics of DNA, physics of molecular motors, mechanics of biological membranes, cell motility and biological networks.

Organizer: Robert Phillips
California Institute of Technology

1:30-1:50 Theory of Polymorphism in Bacterial Flagella
Tom Powers, Brown University

1:55-2:15 Simple Stochastic Models of Motor Protein Dynamics
Anatoly Kolomeisky, Rice University, and Michael Fisher, University of Maryland, College Park

2:20-2:40 Protein Folding as a Search and Optimization Problem
Ken Dill, University of California, San Francisco

2:45-3:05 Cryo-Electron Tomography of Spiroplasma melliferum Reveals theStructural Organization of the Cytoskeleton and Explains Motility
Achilleas Frangakis, California Institute of Technology

Wednesday, May 26

MS58 (For Part II, see MS64)

Dynamics of Microstructure and Defects in Solids: Discrete and Continuum Models: Part I

1:30 PM-3:10 PM

Room: Regency Ballroom B

The motion of defects, such as a phase boundaries, cracks or dislocations,in a crystalline solid is typically associated with energy dissipation at the macrolevel. Phenomenological continuum models of defect dynamics do not fully explain the origin of dissipation and often fail to predict other observed features of defect motion such as lattice trapping. Recent work on direct lattice modeling attributes the macroscopic dissipation to the energy transfer from macro to microscales by short-length lattice waves. A better understanding of this phenomenon and the associated defect kinetics will help to develop more realistic continuum models that capture the important features of the lattice dynamics. The goal of this minisymposium is to bring together scientists working on both discrete and continuum models, with the hope that this interaction will lead to further advances in understanding defect dynamics. The topics of the invited talks range from plasticity and dislocation dynamics to the phase boundary motion and pattern formation.

Organizer: Timothy Healey
Cornell University

Organizer: Anna Vainchtein
University of Pittsburgh

1:30-1:50 Lattice Model of Plastic Deformation
Lev Truskinovsky, Ecole Polytechnique, France

1:55-2:15 Dynamic Transitions in Bistable Lattices
Leonid Slepyan, Tel Aviv University, Israel

2:20-2:40 From Atoms and Defects to Kinetic Relations
Kaushik Bhattacharya, California Institute of Technology

2:45-3:05 Explicit Kinetic Relation from "First Principles"
Lev Truskinovsky, Ecole Polytechnique, France and *Anna Vainchtein*, University of Pittsburgh

Wednesday, May 26

MS59 (For Part III, see MS65)

Challenges in Systems with Nematic and Smectic Order II

1:30 PM-3:10 PM

Room: Regency Ballroom C

Liquid crystals and their fascinating properties have been studied extensively since the 1920s, in particular in the physics and engineering literature. The most successful mathematical approach to the subject is the Ericksen-Leslie theory for nematic liquid crystals proposed in the 60s. Recent progress in the analysis of smectic liquid crystals was based on elasticity models within the framework of the Landau-De Gennes energy.

In the late 1990s, a completely new class of materials - so-called liquid crystal elastomers - was synthesised by cross-linking liquid crystal systems close to their transition temperature from the isotropic to the nematic or smectic phase. The key-feature of these new materials is the coupling of an orientational degree of freedom and the elasticity of the underlying network that is formed in the cross-linking process. The first mathematical theories for a class of nematic elastomers emerged in the past few years and have already substantially contributed to the understanding of the novel properties of these fascinating systems.

Organizer: Chun Liu
Pennsylvania State University

Organizer: Georg K. Dolzmann
University of Maryland, College Park

Organizer: Antonio DeSimone
SISSA/Trieste, Italy

1:30-1:50 Numerical Modeling of Frustrated Nematic Twist Cells
Eugene Gartland, Kent State University and Fulvio Bisi, Riccardo Rosso, and Epifanio Virga, University of Pavia, Italy

1:55-2:15 Smectic Phases with Cubic Symmetry: Layered Systems with High Intrinsic Curvature
Brian DiDonna and Randall Kamien, University of Pennsylvania

2:20-2:40 Homogenization Estimates for Polydomain Nematic Elastomers undergoing to Large Deformation
Pedro Ponte-Castaneda and Martin Idiart, University of Pennsylvania

2:45-3:05 On the Defect Dynamics in Nematic Liquid Crystals
Chun Liu, Pennsylvania State University

Wednesday, May 26

MS60 (For Part II, see MS66)

Recent Developments in Modeling and Simulations of Interface Problems in Materials Science: Part I

1:30 PM-3:10 PM

Room: Regency Ballroom E

Moving interfaces and free boundaries appear in a wide variety of problems in materials science. One of the main difficulties found in this subject is the coupling and interaction of interface dynamics and bulk dynamics at different scales. In this minisymposium, we plan for the dissemination of recent progresses made in modeling and computational methods related to material interfaces found in thin film growth, grain boundary morphology, convection and diffusion of surfactants, dislocation simulations, and other topics. It is our hope to stimulate discussions of the latest results and techniques for the important and challenging subject of interfaces in materials science.

Organizer: Li-Tien Cheng
University of California, San Diego

Organizer: Hongkai Zhao
University of California, Irvine

1:30-1:50 A Kinetic Model for a Step Edge
Russel Caflisch, University of California, Los Angeles

1:55-2:15 A Fourth Order Accurate Discretization for the Laplace and Heat Equations on Arbitrary Domains, with Applications to the Stefan Problem
Frederic Gibou, Stanford University

2:20-2:40 Grain Boundary Diffusion Due to Stress and Electromigration
Jon Wilkening, New York University

2:45-3:05 Level Set Simulations of Dislocation-particle Bypass Mechanisms
Yang Xiang, Hong Kong University of Science and Technology, Hong Kong

Wednesday, May 26

MS61 (For Part I, see MS55)

Crack Propagation in Elastic and Viscoelastic Solids: Part II

1:30 PM-3:10 PM

Room: Regency Ballroom D

The minisymposium addresses the analytical and experimental studies of subsonic and transonic crack propagation in elastic and viscoelastic bodies. Evidence of shear crack propagation in excess of the shear wave speed has been provided from observations of shallow crustal earthquakes and confirmed by recent experiments. The study of this phenomenon requires the design of new fracture criteria, finding fundamental solutions to the associated fracture problems, and developing new methods for matrix Wiener-Hopf factorization. Recent results in this area including the analysis of out-of plane corrugation waves and new experimental data on sub-Rayleigh and supershear rupture will be reported.

Organizer: Jay R. Walton
Texas A&M University

Organizer: Yuri A. Antipov
Louisiana State University

1:30-1:50 Dynamic Steady-state Crack Propagation in Anisotropic Viscoelastic Material
Jay R. Walton, Texas A&M University

1:55-2:15 Wave of Transition in Chains and Lattices from Bistable Elements
Andrej V. Cherkaev and Elena Cherkaev, University of Utah and Leonid I. Slepyan, Tel Aviv University, Israel

2:20-2:40 A Solution Method for Dynamically Accelerating Cracks in Viscoelastic Materials and Elastic Bimaterials
Tanya Leise, Rose-Hulman Institute of Technology

2:45-3:05 High Order Asymptotics and Perturbation Problems for 3D Interfacial Cracks
Yuri A. Antipov, Louisiana State University

Wednesday, May 26

MS62 (For Part I, see MS56)

Mathematical Modeling of Electrochemical Systems: Part II

1:30 PM-3:10 PM

Room: Regency Ballroom F

Many modern materials processing techniques are based on electrochemical processes. This minisymposium is devoted to mathematical models, methods and approaches used for investigation of electrochemical processes relevant to materials science, especially to nanotechnology. The speakers will present recent results on mathematical modeling of such electrochemical phenomena as anodic dissolution, electrodeposition, electroconvection, electrocapillary and electrokinetic effects, electrophoresis, etc.

Organizer: Alexander A. Golovin
Northwestern University

1:30-1:50 Ion Exchange Funneling
Isaak Rubinstein and Boris Zaltzman, Ben-Gurion University, Israel

1:55-2:15 Electroconvection in Concentration Polarization
Boris Zaltzman and Isaak Rubinstein, Ben-Gurion University, Israel

2:20-2:40 Fluid Flow and Dispersion in the Electrophoretic Separation of Biomolecules
Sandip Ghosal, Northwestern University

2:45-3:05 Electrokinetic Phenomena Due to AC Faradaic Charging
Hsueh-Chia Chang and Yuxing Ben, University of Notre Dame

Coffee Break

3:10 PM-3:40 PM

Room: Regency Foyer

Wednesday, May 26

MS63 (For Part II, see MS57)

Quantitative Modeling in Biology: Part III

3:40 PM-5:20 PM

Room: Regency Ballroom A

The advent of single molecule techniques has opened up the possibility of a new generation of mathematical modeling in the biological sciences. The aim of this symposium is to provide examples of the types of experiments being done in this field and of the mathematical models being put forth to greet them. Some of the particular examples to be included are: mechanics of DNA, physics of molecular motors, mechanics of biological membranes, cell motility and biological networks.

Organizer: Robert Phillips
California Institute of Technology

3:40-4:00 The Noisy Machine: Stochasticity in Gene Regulation
Michael Elowitz, California Institute of Technology

4:05-4:25 Precise Measurements - and Theory - of Elasticity and Strengthin Ultra Thin Biomembranes
Evan Evans, University of British Columbia, Canada; Volkmar Heinrich, Boston University

4:30-4:50 Analytic Models for Mechanotransduction: Gating a Mechanosensitive Channel
Paul Wiggins, California Institute of Technology

Wednesday, May 26

MS64 (For Part I, see MS58)

Dynamics of Microstructure and Defects in Solids: Discrete and Continuum Models: Part II

3:40 PM-5:20 PM

Room: Regency Ballroom B

The motion of defects, such as a phase boundaries, cracks or dislocations,in a crystalline solid is typically associated with energy dissipation at the macrolevel. Phenomenological continuum models of defect dynamics do not fully explain the origin of dissipation and often fail to predict other observed features of defect motion such as lattice trapping. Recent work on direct lattice modeling attributes the macroscopic dissipation to the energy transfer from macro to microscales by short-length lattice waves. A better understanding of this phenomenon and the associated defect kinetics will help to develop more realistic continuum models that capture the important features of the lattice dynamics. The goal of this minisymposium is to bring together scientists working on both discrete and continuum models, with the hope that this interaction will lead to further advances in understanding defect dynamics. The topics of the invited talks range from plasticity and dislocation dynamics to the phase boundary motion and pattern formation.

Organizer: Timothy Healey
Cornell University

Organizer: Anna Vainchtein
University of Pittsburgh

3:40-4:00 A Global Bifurcation Approach to Two-Phase Equlibria in Elastic Solids
Timothy Healey, Cornell University

4:05-4:25 A Probabilistic Approach to Transient Pattern Formation
Thomas Wanner, George Mason University

4:30-4:50 Travelling Waves in a Discrete Chain with Bi-stable Springs: A Model for Martensitic Solids
Prashant Purohit and Kaushik Bhattacharya, California Institute of Technology

4:55-5:15 Dispersion, Dissipation and the Kinetic Relation for a Dislocation
Basant Sharma and Phoebus Rosakis, Cornell University

Wednesday, May 26

MS65 (For Part II, see MS59)

Challenges in Systems with Nematic and Smectic Order III

3:40 PM-5:20 PM

Room: Regency Ballroom C

Liquid crystals and their fascinating properties have been studied extensively since the 1920s, in particular in the physics and engineering literature. The most successful mathematical approach to the subject is the Ericksen-Leslie theory for nematic liquid crystals proposed in the 60s. Recent progress in the analysis of smectic liquid crystals was based on elasticity models within the framework of the Landau-De Gennes energy.

In the late 1990s, a completely new class of materials - so-called liquid crystal elastomers - was synthesised by cross-linking liquid crystal systems close to their transition temperature from the isotropic to the nematic or smectic phase. The key-feature of these new materials is the coupling of an orientational degree of freedom and the elasticity of the underlying network that is formed in the cross-linking process. The first mathematical theories for a class of nematic elastomers emerged in the past few years and have already substantially contributed to the understanding of the novel properties of these fascinating systems.

Organizer: Chun Liu
Pennsylvania State University

Organizer: Georg K. Dolzmann
University of Maryland, College Park

Organizer: Antonio DeSimone
SISSA/Trieste, Italy

3:40-4:00 Effect of Random Field Disorder on N-I Transition
Banahalli Ratna, Naval Research Laboratory

4:05-4:25 Disclinations in a Homogeneously Deformed Nematic Elastomer
Eliot Fried, Washington Univeristy, St. Louis

4:30-4:50 Landau-de Gennes Model of Liquid Crystals and Critical Wave Number
Xingbin Pan, National University of Singapore, Republic of Singapore

4:55-5:15 Analytic Aspects of Phase Transitions in Liquid Crystals
Daniel Phillips and Patricia Bauman, Purdue University; Maria Carme Calderer, University of Minnesota, Minneapolis; and Chun Liu, Pennsylvania State University

Wednesday, May 26

MS66 (For Part I, see MS60)

Recent Developments in Modeling and Simulations of Interface Problems in Materials Science: Part II

3:40 PM-5:20 PM

Room: Regency Ballroom D

Moving interfaces and free boundaries appear in a wide variety of problems in materials science. One of the main difficulties found in this subject is the coupling and interaction of interface dynamics and bulk dynamics at different scales. In this minisymposium, we plan for the dissemination of recent progresses made in modeling and computational methods related to material interfaces found in thin film growth, grain boundary morphology, convection and diffusion of surfactants, dislocation simulations, and other topics. It is our hope to stimulate discussions of the latest results and techniques for the important and challenging subject of interfaces in materials science.

Organizer: Li-Tien Cheng
University of California, San Diego

Organizer: Hongkai Zhao
University of California, Irvine

3:40-4:00 A Two-Dimensional Finite Element Method for Simulating Microstructure and Constitutive Response of Polycrystals During High Temperature Plastic Deformation
Allan Bower, Brown University

4:05-4:25 Adaptive simulation of Microstructured Materials: Multiphase Flows
John Lowengrub, University of California, Irvine

4:30-4:50 An Efficient Method for Tracking Interfaces in 3D Homogeneous Media
Xiaofan Li, Illinois Institute of Technology

4:55-5:15 Numerical Methods for Material Transport with Global Dynamics
Hongkai Zhao, University of California, Irvine

Conference adjourns

Notes

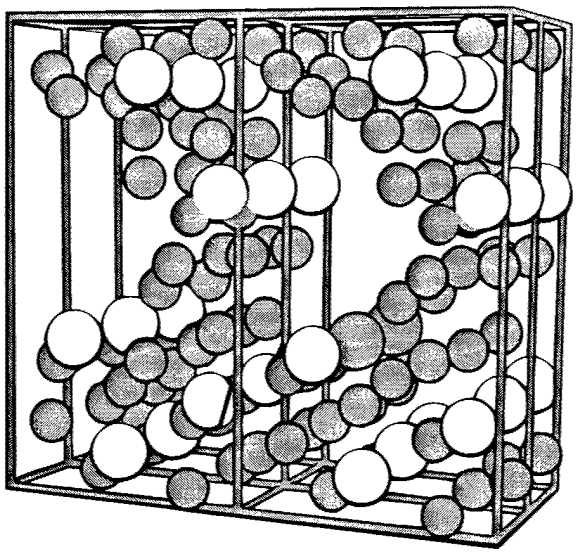
Abstracts

SIAM Conference on Mathematical Aspects of

MATERIALS SCIENCE

May 23-26, 2004

Hyatt Regency Los Angeles
at Macy's Plaza
Los Angeles, California



All abstracts published as submitted by the authors.

MS1

New Exact Results for the Effective Electric, Elastic, Piezoelectric and other Properties of Composite Ellipsoid Assemblages

Composite ellipsoid assemblages made up of two-phase confocal ellipsoidal particles are considered. Information of exact nature is sought on the effective behaviour of this microstructure in the setting of a variety of physical phenomena. A unified formalism is developed which is based on an inhomogeneity problem whose solutions for the fields are linear combinations of the fields which solve the conductivity problem. The procedure results in a set of exact relations between the effective moduli. The complete set of the effective moduli is available only in some instances.

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MS1

Bounds for Conducting Networks

We compute exact bounds for mixtures of two types of linear resistors on a square conducting lattice with given proportions. We compare the result with the analog G-closure problem on the continuum highlighting qualitative and quantitative differences.

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MS1

The G-closure Problem: The Geometric Approach

A polycrystal is a mixture of anisotropic materials (crystals) where each material may participate in a composite in any orientation. The effective conductivity tensor of such a composite depends on the microstructure of the composite. The set of effective properties one can obtain by mixing the same set of materials in different ways is called the G-closure of the original materials. The G-closure set has two important qualities: SO(3) invariance and a certain convexity property. The difficulty here is that SO(3) invariance and convexity hold in different coordinate systems. In this talk we show that it is possible to combine both properties to obtain non-trivial results. The goal of this talk is to alert the composites community to a new way of attacking the general G-closure problem.

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MS1

Cross Properties for Multiphase Composites

We study the coupling between two different effective properties, such as thermal conductivity and magnetic permeability for a medium made of several isotropic phases. In two dimensions, for two phases, such a set is known. (Work of Bergman, Milton and Cherkaev-Gibiansky). We explore two and three dimensions and several phases using a new code implementing the compensated compactness approach. In two dimensions, for three or more phases, quasiconformal mappings play an interesting role.

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MS2

Ferroelectric Phases of Chiral Smectic C Liquid Crystals

Chiral smectic C liquid crystals (smectic C*) may present ferroelectric phases. These are characterized by the strong coupling between the material polarization and applied electric fields, allowing for the manufacturing of fast switching display devices. Motivated by Doi's theory of nematic polymers, we develop and analyze kinetic theory models of ferroelectricity of smectic C* liquid crystals. We show that static ferroelectric configurations appear as Hopf bifurcation states of higher temperature (Smectic A) fields, and analyze a time-dependent model of switching.

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MS2

A Mathematical Overview on Micro-macro Models for Complex Fluids

We will introduce the so-called micromacro models used in the simulation of of polymeric fluid flows. These models couple through the stress tensor the Navier Stokes equations with some stochastic differential equations which rule the evolution of the configuration of the polymers in the flow. Such a coupling raise many mathematical questions related to existence and uniqueness of solutions, convergence of approximation schemes, and so forth. We will overview some recent progress in the field.

Claude Le Bris
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MS2
Numerical Analysis of Polymeric Fluid Flows

The talk will focus on some numerical aspects of the simulation of micro-macro models of polymeric fluids. These models couple through the stress tensor the Navier Stokes equations with some stochastic differential equations which rule the evolution of the configuration of the polymers in the flow. We will present a convergence analysis in a simple case, as well as some questions raised by the correlation in space of the noise. Alternative approaches to discretize this coupled system will also be presented.

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MS2
Some Theoretical Results for the Dumbbell Model of Polymeric Fluids

I will give a short review about some new theoretical results for the dumbbell model of polymeric fluids, especially focusing on the well-posedness and numerical analysis results. The mathematical formulation and the multiscale numerical scheme CONNFFESSITE and BCF for the dumbbell model is introduced at first, both the SDE form and the Fokker-Planck equation are involved. We then introduce our work on the well-posedness results of the SDE and FPE, and the numerical analysis of the BCF in high dimension. Some related works are also refered.

Tiejun Li
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MS2
Moment Closure and Numerical Simulations of a Complex Fluid Model

In this talk, we give a new moment closure for the FENE model for polymeric materials. The new system still possess an energy dissipation law. We prove the local existence of solutions to the closure equation. Some numerical comparison results between the macroscopic closure system and the Monte-Carlo simulation to the original micro-macro coupled system are presented.

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MS3
Finite-Temperature Micromagnetic Simulations of Magnetization Reversal

Numerical micromagnetics is a useful paradigm for studying the dynamics of magnetization reversal of single-domain, nanoscale magnets. While modeling a nanomagnet may require only 10^5 computational elements, this is computationally challenging since long-ranged dipole-dipole interactions between elements cannot be neglected. However, simulations lasting tens of nanoseconds are possible using sophisticated strategies like the Fast Multipole Method. The simulations are used to investgate interesting dynamical phenomena at finite-temperature and can be compared with experiments.

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MS3
Motion of Magnetic Domain Walls in Thin, Narrow Strips

In thin, narrow strips of ferromagnetic material, magnetic domains orient parallel to the long axis of the strip. In-plane transverse walls form at the junction between oppositely directed domains. Micromagnetic simulations show that a magnetic field applied along the strip axis induces domain wall motion primarily through precession about the strip demagnetizing fields. A simple model is presented that quantitatively agrees with results from the full micromagnetic model, including domain wall momentum and retrograde motion.

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MS3
Micromagnetics Simulations in Multilayers

A multilayer consists of two or more magnetic films, separated by a layer of non-magnetic material. Multilayers seem to have good permanent magnet properties, and in particular, a high coercive field, and an approximately rectangular hysteresis loop. For that reason, multilayers are an integral part of magnetic memories (MRAMs), and have been one of the most important applications of ferromagnetic materials in the past few years. In this talk, I will present a new model for the study and simulation of the magnetization reversal process in double layers. A comparison with traditional 3D simulations will be presented.

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MS3
Micromagnetic Simulations of Demagnetization Curves for the Nanocrystalline PrFeB Magnets

The Gauss-Seidel projection method is used to calculate the demagnetization curves for the single-phase nanocrystalline PrFeB magnet. It is observed that magnetic reversal for PrFeB magnet starts near the grain boundary where the angle between the external magnetic field and easy direction of the magnet can be as large as 90^o. We also calculated the demagnetization curves, coercivity $\mu_{0i}H_c$ and remanence J_r for different temperatures. The numerical

results are consistent with the experimental observations.

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MS4

Phase-field Modeling of Morphological Evolution in Thin Films

A phase-field model is developed to study the morphological instability of a thin film as well as the phase separation process in a binary film leading to the formation of quantum dot structures. An efficient iterative method is proposed to solve the mechanical equilibrium equation for a thin film in the presence of both misfit dislocations and substrate constraint. The dependence of quantum dot morphologies and spatial arrangement on the substrate constraint and the misfit dislocation distribution is investigated.

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MS4

Analytical and Numerical Methods for Studying Phase Transformations in Compositionally Stressed Thin Films

We investigate the role of elastic stresses on diffusional phase transformations in multi-component solid thin films. The elastic stresses results from compositional misfit between different components, mechanical attachment to a compliant substrate and applied external loadings. The stresses are found by using an analytic solution to the elasticity problem based on the Laplace transform. This method can be applied to isotropic and anisotropic films, and to free standing films and films attached to a substrate. The diffusion problem, with elasticity, is formulated based on a Cahn-Hilliard equation, and is solved numerically using a second order semi-implicit unconditionally stable finite difference method. Elastic stresses can have a large effect on film morphology depending on sytem parameters.

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MS4

Computational Modelling of Microstructure Evolution

We provide a brief overview of the methods used in computational modelling of microstructure evolution to set the stage for the minisymposium. The discussion will be centered around phase-field and boundary integral/element methods where elastic stress plays a role. We consider the factors leading to surface stress effects in phase-field models and present recent results from three-dimensional phase-field simulations for systems with highly anisotropic surface energy.

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MS5

The Bifurcation of Periodic Solutions of the Ginzburg-Landau Equations near a flat wall

The Ginzburg-Landau equations in a half-plane are considered in the large κ limit. We look at the reduced set of equations obtained in that limit. It is proved that the one-dimensional solution presented by Pan undergoes a series of bifurcations which can start at applied magnetic field values which are lower than H_{C_2}. We than classify the bifurcating modes and show that they all tend to be periodic away from the boundaries.

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MS5

Ginzburg-Landau Minimizers with Prescribed Degrees in Perforated Domains. Capacity of the Domain and Emergence of Vortices.

Let Ω be a 2D domain with holes $\omega_0, \omega_1, \ldots, \omega_j, j = 1...k$. In domain $A = \Omega \setminus \left(\cup_{j=0}^{k} \omega_j \right)$ consider class $\mathcal{J}$ of complex valued maps having degrees 1 and -1 on $\partial\Omega$, $\partial\omega_0$

respectively and degree 0 on $\partial\omega_j, j = 1...k$. We show that if $\text{cap}(A) \geq \pi$, minimizers of the Ginzburg-Landau energy E_κ exist for each κ. They are vortexless and converge in $H^1(A)$ to a minimizing S^1-valued harmonic map as the coherency length κ^{-1} tends to 0. When $\text{cap}(A) < \pi$, we establish existence of quasi-minimizers, which exhibit a different qualitative behavior: they have exactly two zeroes (vortices) rapidly converging to ∂A.

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MS5
Vortex Filaments in Bose-Einstein Condensates

I will discuss some theorems proving the existence large numbers of local minimizers of the Gross-Pitaevsky functional, which is essentially a nonhomogeneous Ginzburg-Landau type functional with an additional term relating to angular momentum. These results are interpreted as proving the existence of stable vortex filaments in rotationally forced Bose-Einstein condensates in certain parameter regimes.

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MS5
Ginzburg-Landau Models on Thin Spherical Shells

For mesoscopic superconductors, it is known that sample goemetry and sample topology greatly affect the material properties. In this talk, we discuss the vortex nucleation in a thin superconducting hollow sphere. The problem is studied using a simplified system of Ginzburg-Landau equations. We present numerical algorithms which preserve the discrete gauge invariance. The discretization is based on a spherical centroidal Voronoi tessellation which offers a very effective high resolution mesh on the sphere for the order parameter, the supercurrent and the induced magnetic field. Various vortex configurations and energy diagrams are computed.

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MS6
Perfectly Plastic Heterogeneous Materials

We consider heterogeneous materials with elastic-perfectly plastic pure phases. Our goal is to evaluate the strength domains of these materials (i.e. the set of stresses that these materials can withstand). We will present our results on the two-dimensional problem that results if the microstructures are compatible with the applied anti-plane deformations.

Guillermo Goldsztein
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MS6
Self-consistent Variational Approach to Anisotropic Nonlinear Conducting

In the framework of the "standard" self-consistent variational effective-medium theory, we consider the problem of binary conducting composites where each phase obeys a power-law behavior with same exponent. By systematically studying the coupling between strong non-linearity and anisotropy, be it due to an underlying lattice or to an intrinsic anisotropy of the constitutive law, we point out non-trivial predictions, but also limitations of the "standard" variational approach.

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MS6
The Influence of Fluctuations in Volume Fraction on the Effective Properties of Nonlinear Composites

Two-phase nonlinear composites with three well-separated length scales are considered. These composites appear as locally homogeneous at the intermediate scale where they a nonuniform distribution of the volume fraction. When the fluctuations in volume fraction are small an expansion of the macroscopic potential can be obtained in terms of the amplitude of the fluctuations. These expansions imply, as a cross-result, necessary conditions on bounds for the effective potential of two-phase nonlinear composites.

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MS6

Higher-order Bounds for Constitutive Relations of Nonlinear Composites

An approach that was initiated by G.W. Milton and S.K. Serkov bounds the constitutive relation of a nonlinear composite by developing a lower bound for the characteristic function of the set, in stress–strain space, on which the constitutive relation is satisfied. This approach is developed further, to permit the deduction of bounds which have a close relation with the classical Hashin–Shtrikman energy bounds, and also bounds which make allowance for higher-order correlations, or for any other morphological information which can be incorporated in the corresponding energy bounds. The theoretical structure will be outlined and examples presented.

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MS7

Diffuse-interface Simulations of Two-phase Flows of Complex Fluids

Two-phase systems of microstructured complex fluids are an important class of engineering materials, coupling three disparate length scales: molecular conformation inside each component, mesoscopic interfacial morphology and macroscopic hydrodynamics. In this paper, we propose a diffuse-interface approach to simulating the flow of such materials. We will outline the general approach for any two-phase complex fluids, and then present several examples including shear-induced deformation, head-on collision and coalescence of drops, and drop retraction.

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MS7

Flow-induced Structures and Property Relationships in Nano-composite

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MS7

Adaptive Mesh Refinement for Complex Fluids

Adaptive mesh refinement is used to compute flows consisting of "complex" fluids. These flows can exhibit multiple spatial and temporal scales. e.g. density and viscosity can jump at material interfaces. Also, surface waves can move much more rapidly relative to the velocity of the underlying flow. In this scenario, the timestep in the vicinity of the moving boundary is much smaller than in the rest of the flow.

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MS7

Multiscale Approach to Flows of Liquid Crystal Polymers

In this talk, I will give an overview of the theories for flows of liquid crystal polymers from the continuum theories such as the classical Ericksen-Leslie theory to the mesoscopic density function theory and the multiscale kinetic theory. I will survey the model predictions in simple shear and elongational flows and identify the issues need to be addressed.

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MS8

A New Regime for Critical Fields

The known destabilizing modes for ferromagnetic samples are coherent rotation, buckling and curling. In the case of an isotropic, cartesian thin film of infinite extension in the direction of the external field a new regime occurs.
This regime results from the weakening of magnetization divergences and displays a correspondingly oscillating behaviour. The oscillation wavelength sets a new lengthscale, resulting from the three lengthscales d, l and t.

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MS8

Simulating ferromagnetic nanostructures with finite elements

The magnetic properties of nanoscaled soft-magnetic particles depend sensitively on their shape. In order to study the subtle shape and size dependence, the techniques to fabricate sub-micron sized ferromagnetic particles of well-defined shape have made remarkable progress in the last years. To name a few examples: ferromagnetic rings, discs and pillars of up to some hundred nm size have recently been investigated intensively by several groups. Understanding magnetization processes in such magnetic nanostructures requires accurate numerical simulation methods. Finite-difference schemes are the most frequently applied methods for micromagnetic simulations. These methods, however, suffer from a reduced accuracy when simulating particles with curved boundaries or inclined facets. The finite element method is still an uncommon technique in micromagnetism, although it provides both the accuracy and the geometrical flexibility that is required to perform reliable numerical simulations in modern magnetic nanostructures of general geometry. In this talk I will outline the mathematical background of a micromagnetic finite-element algorithm and present several examples on simulations of static and dynamic magnetization processes in soft-magnetic nanostructures.

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MS8

2-D Stability of Nel Walls

Magnetic domains are separated by a large variety of transition layers (domain walls). The dominating domain wall in thin films is the so called Néel wall, which has a one-dimensional structure. Another wall type is the two-dimensional cross-tie-wall. We want to show non-linear stability of the one-dimensional Néel wall in a certain parameter regime. Mathematically this means analyzing a two-dimensional variational problem and showing that the one-dimensional minimizer is asymptotically optimal.

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MS8

Numerical Methods for the Micromagnetic Simulation of the Entire Recording Process

We present numerical methods for 3D micromagnetic simulation of the entire recording process of a bit on a granular media. The magnetization processes in the yoke and gap regions are treated by a hybrid FEM/BEM method. The use of hierarchical matrices reduces the required CPUtime by a factor of 10. The interaction between the moving head and media can be treated by a field box. As the box moves together with the head we have to compute the head-media interaction matrix only once.

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MS9

Microstructure and Coarsening Kinetics of Ordered Precipitates in Ni-Base Alloys: Comparison between Experimental Results and Modeling

Many features of Ni_3Al precipitate microstructures in Ni-Al alloys have been captured beautifully by computer modeling experiments, and some important aspects of kinetic behavior have been successfully reproduced. Modeling of the coarsening behavior of Ni_3X precipitates in other Ni-X alloys (X = Ga, Ge, Si and Ti) has not been as successful. Experimental and computational models of Ni_3X precipitate microstructures and kinetics will be compared, and targets for future modeling experiments will be presented.

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MS9

Phase Field Modeling: A Quantitative Application to Phase Transformations in Ni-based Superalloys

We present a quatitative phase field modelling of microstructural evolutions in alloys. The method is illustrated through the specific case of Ni-based alloys, where we examine the precipitation processes of $\gamma\prime$ particules as a function of the thermal treatment.

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MS9

Nucleation in Phase Field Methods

Using phase field models as a predictive tool in materials science is today mainly limited by the ability of controling the first stages of the microstructural evolution. The aim of the present work is to show how and to what extend the addition of a stochastic Langevin noise allows the quantitative description of the nucleation stage.

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MS9

The Role of Heterogeneities in Solidification: A Dirt-dynamics Duality

Phase field models of solidification can be extended to include polycrystalline effects by the addition of a single new order parameter characterizing the orientation of the crystal (in two dimensions). In this presentation we discuss some of the variety of phenomena which can now be explained within the context of this simple modification, and examine future areas for broadening the model's applicability.

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MS10

Fractional Degree Vortices for a Spin-coupled Ginzburg-Landau System

Recent papers in the physics literature have introduced spin-coupled (or spinor) Ginzburg-Landau models for complex vector-valued order parameters in order to account for ferromagnetic or antiferromagnetic effects in high-temperature superconductors and in optically confined Bose–Einstein condensates. In this note we observe that such models can lead to new types of vortices, with fractional degree and non-trivial core structure.

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MS10

Location and Bending of Vortex Lines in Three Di-

mensional Domains

In a joint work with del Pino and Felmer we find for all small ε a solution u_ε to Ginzburg-Landau equation with zero Neumann boundary conditions in $\Omega \subset \mathbf{R}^3$. The zero level set of u_ε is a straight line segment Γ which represents a nondegenerate critical point of length of curves with endpoints on $\partial\Omega$. The distance of the vortex filament to Γ is $O(1/\log\frac{1}{\varepsilon})$.

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MS10

Surface Superconductivity of Type II Superconductors in 3 Dimensions

We investigate superconductivity of a type II superconductor occupying a 3-dimensional bounded domain, and improve the existing estimate of the upper critical field H_{C_3}. We also analyze the concentration behavior of the order parameters for a sample subjected to an applied magnetic field lying in between H_{C_2} and H_{C_3}.

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MS10

Vortices in the Ginzburg-Landau Model of Superconductivity in the Large Kappa Limit

We will give a review of various recent results obtained on the statics and dynamics of vortices in the Ginzburg-Landau model.

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MS11

Stability of Composite Materials with Inclusions of Negative Stiffness

Negative stiffness entails a reversal of the usual directional relationship between force and displacement in deformed objects. Of course an isolated object with negative stiffness is unstable. But incremental negative stiffness can be achieved in some materials. Examples are (1) a column buckled into an S shape, (2) flexible tetrakaidecahedra (models of single cells in foams) deformed in compression under displacement control, and (3) ferroelastic domains in the vicinity of a phase transition. Analysis discloses peak damping and large stiffness anomalies are possible in viscoelastic composites with inclusions of negative stiffness. An experimental illustration discloses singular mechanical damping tan delta in a lumped unit cell system containing post-buckled polymeric elastomer tubes. A further experimental illustration of extreme behavior showed composites prepared with a dilute concentration of ferroelastic inclusions (vanadium dioxide) exhibited large peaks in tan delta and anomalies in dynamic modulus. These results point to the possibility of achieving extreme behavior in designed composites. We report analysis of extreme thermal expansion and piezoelectric coefficients in thermoelastic and piezoelectric composites. We examine the stability of a lumped system and show that extreme mechanical damping is possible within the regime of stability according to the Routh Hurwitz method.

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MS11

Effective Behavior, Field Fluctuations and Loss of Ellipticity in Hyperelastic Composites

The "second-order" method, which makes use of "generalized" secant moduli depending on both the averages and second moments of the field fluctuations within the context of a "linear comparison composite," is used to estimate the effective behavior of hyperelastic composites subjected to finite deformations. Applications are given for porous elastomers. The accuracy of the method is studied by comparison to bounds and other rigorous information, and the implications for loss of ellipticity are considered.

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MS11

Propagation and Lozalisation of Waves in High Contrast Periodic Media and Photonic Crystals

The effect of band gaps is used for example in photonic/phononic crystals. In the "resonance" regime, the band gaps are characterized explicitly asymptotically for high contrast phases, using tools of "non-classical" homogenization. We show that for a gap frequency the solution is localised and its explicit asymptotics decays exponentially at infinity. Error bounds are given. We address also the question of the existence of eigenmodes in waveguides in periodic media.

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MS11

Homogenization and Stability in Nonlinear Solids with Periodic and Almost Periodic Microstructures

The influence of the scale size on the stability of finitely strained, rate-independent nonlinear solids with periodic microstructures is analyzed using a multiple scales asymptotic technique. The proposed general theory is applied to the investigation of the micro- and macro-failure surfaces in periodic solids of infinite extent. Applications are presented for an aluminum honeycomb, for which careful experimental data are available. The periodic solid's failure

surfaces are upper bounds for the failure of their imperfect counterparts.

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MS12
Dynamics of Ferroelectric Phases of Liquid Crystals

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MS12
Numerical Modeling of Periodic Structures in Liquid Crystal Films

Periodic structures are common in liquid-crystal films. This is true for systems involving chiral molecules, which have intrinsic periodic tendencies, as well as for achiral systems (such as nematics), which do not. In technologies such periodic patterns can be desirable (in diffractive optics applications, for example) or not. In any case, they can be challenging to model numerically. We report on our experience with two systems. The first involves a "stripe phase" that can appear in a nematic in a magnetic field in the "bend-Freedericksz geometry." The second involves a cholesteric material with negative dielectric anisotropy in an applied electric field.

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MS12
On Multiscale Effects in Viscoelaticity

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MS12
Accurate Numerical Simulations of Nematic Polymers in Shear Flow using

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MS13
Cross-Tie Walls in Soft Ferromagnetic Films

Recent results on the structure of cross-tie walls in soft ferromagnetic films are presented. This is joint work with R.V. Kohn, S. Mueller, and F. Otto.

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MS13
Schrdinger Maps and Landau-Lifshitz Equations

The Landau-Lifshitz equation without damping is a specific case of the Schrödinger maps problem, a geometric and highly nonlinear generalization of Schrödinger's equation. I will present a proof of local existence and uniqueness of the Cauchy problem in Sobolev spaces of high enough order. This result also holds when Landau-Lifshitz is coupled to a magnetic field satisfying stationary Maxwell's equations. In addition, with certain symmetry assumptions, we have well-posedness in the critical Sobolev spaces.

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MS13
Domain Wall Motion in Ferromagnetic Layers

We consider the dynamics of one-dimensional micromagnetic domain walls in layers of uniaxial anisotropy. In the regime of bulk materials, i.e. when the thickness is assumed to be infinite, and the magnetostatic interaction terms appear as local quantities, explicit traveling wave solutions for the corresponding Landau-Lifshitz equation, known as Walker exact solutions, can be constructed. A natural question is whether this construction can be perturbed to the non-local regime of layers of finite thickness. The stability analysis that I will present gives an affirmative answer.

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MS13
Boundary Vortices for Thin Ferromagnetic Films

We consider a simplified version of the micromagnetic energy for thin films of ferromagnetic materials. We study critical points and solutions of the Landau-Lifshitz equation associated to this energy. In particular we determine their asymptotic behavior in the thin film limit. The asymptotic regime we consider gives rise to Ginzburg-Landau-type vortices.

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MS14
The Effect of Inhomogeneity on Microstructure Evolution

The equilibrium shapes of an isolated precipitate in infinite matrix are found via dynamic simulation of the diffusional transformation. We discuss the relationship between the dimensionless concentration at equilibrium and the effective particle size, and its implication on the coarsening theory. The effect of inhomogeneity on the equilibrium states will be addressed. The results will be shown in both two

and three-dimensional cases.

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MS14

Controlling the Shape of Growing 3D Crystals and Supression of the Mullins-Sekerka Instability

In this talk, we consider the quasi-steady evolution of growing crystals in 3-D. A reexamination of this problem reveals that the Mullins-Sekerka instability may be suppressed by appropriately varying the undercooling (far-field temperature) in time. For example, in 3-D, by imposing the far-field temperature flux (rather than a temperature condition), we demonstrate that there exist critical conditions of flux at which self- similar or nearly self-similar nonlinear evolution occurs and the shape is dominated by a given mode leading to non-spherical, nearly shape invariant growing crystals. This result was predicted by our previous linear analysis and suggests that our theory is applicable to real physical systems. We provide a simulation of a physical experiment that could be carried out in a laboratory in which a desired shape of a crystal is achieved and maintained during growth by appropriately prescribing the far-field heat flux. This work has important implications for shape control in processing applications.To simulate the problem numerically, we use a boundary element method with a fully adaptive surface triangulation. This enables us to simulate 3-D crystals stably and accurately well into the nonlinear regime. This work is joint with Dr. Vittorio Cristini (Dept. Math, Dept Biomed Eng. UCI)

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MS14

Dynamics of Precipitates in Three-dimensional Elastic Media

In this talk, the dynamics of precipitate evolution in elastically stressed solids are discussed through numerical simulations of both sharp interface models and diffuse interface models. In particular, we will study the effect of anisotropic surface energy, the formation of a concave precipitate, and merging of precipitates.

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MS14

Modeling Effects of Stress on the Evolution of Polycrystalline Microstructures

The analysis simulates the evolution of crystallographic transformations in polycrystalline materials by combining microstructural evolution with macroscopic properties of materials when the thermodynamic formalism of phase-field grain boundary and theory of martensitic phase transformation are considered. Both microstructural phase transformation and grain boundary evolution are affected by internal (residual) stresses developed as a result of crystal defects. The model treats the effect of local stresses on microstructural development during transformations and grain growth.

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MS15

Ginzburg-Landau Equation in a Thin Domain

We study the GL equation with magnetic effect in a thin domain, which has variable thickness. This problem reduces to the equation on a low-dimensional domain with variable coefficient. We relate the problem on a thin domain with solution structure.

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MS15

Phase Patterns of the Ginzburg-Landau Equation with Discontinuous Coefficients in a Ring

We consider the Ginzburg-Landau equation with a piecewise constant coefficient in a ring. This coefficient represents the variable thickness of a conductor and it allows a number of thin regions. Namely this is a simplified model of a S-c-S junction with multi constrictions. We prove the existence of solutions with non-uniform phase pattern. Moreover in the limit of the GL parameter we show the configuration of the phase pattern explicitly.

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MS15
The Zero Set of the Order Parameter

We review recent work on the zero set of the order parameter in two dimensions. We provide theoretical and experimental support for certain forms of the zero set. We also examine recently published theoretical predictions for new forms of the zero set, and show that they are incosistent with basic results from calculus of variations.

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MS15
A Comparison of Models for SNS Junctions via Ginzburg-Landau Theory

We will explore various models for the transmission of a supercurrent across a thin section of normal material, basing our approach on Ginzburg-Landau theory. We will also look into modeling of "weaklinks" in which a superconducting sample is severely constricted in some thin region. Focus will be placed on capturing the relationship between the current and the jump in the phase across the junction or link. The analysis is based on an asymptotic study of the energy via Gamma-convergence techiques.

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MS16
Can We Find the Structure of a Composite From its Effective Properties?

The problem of characterizing the microstructure of a composite material is reduced to reconstruction of the spectral function which contains all information about the structure. The spectral function can be uniquely recovered from the Stieltjes representation using effective complex permittivity of the composite material measured in an interval of frequency. Self-adjointness of the operator is used to formulate a stable reconstruction problem for the non-decreasing spectral measure. Classes of composites are discussed that admit unique reconstruction of the microgeometry.

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MS16
Slowing Down the Light by a Photonic Crystal

Consider electromagnetic wave incident on the surface of semi-infinite photonic crystal. At certain frequencies, the wave can slow down dramatically after entering the periodic medium. Usually, a significant slow-down is accompanied by nearly total reflection, which implies that only a tiny portion of the incident radiation is converted into the slow mode (this is always the case at frequencies near photonic band edges). We demonstrate that if the frequency lies in the vicinity of a stationary inflection point of dispersion relation, one can simultaneously achieve an arbitrarily low group velocity of light and nearly total conversion of incident radiation into the slow electromagnetic mode. We also formulate the conditions, under which the electromagnetic dispersion relation of photonic crystal can develop a stationary inflection point.

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MS16
Phononic Band Gap Structures and Localised Eigen-States

We consider a spectral problem for the Lamé operator in a doubly periodic composite medium. The aim of the work is to study the structure of the spectrum and to analyse the Bloch waves "propagating" within such a structure. It is well-known that there are "gaps" within the spectrum, i.e. within certain intervals of frequencies the elastic waves of certain type and polarization do not not propagate through the composite medium. It is also important to be able to design composites that possess stop bands within a certain frequency range. These questions are addressed in the lecture. In addition, we consider analysis of defect modes associated with localised eigen-states for a composite containing "defects" periodically distributed on the plane. Applications are considered in problems of design of passive mass dampers and elastic/optical wave guides.

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MS16
An Analytic Model of Composites with Locally Resonant Units

A simple analytic model is presented for three-component composites that exhibit local resonance behavior. We show that the effective elastic constants can turn negative. Expressions for the effective elastic constants are derived for both three dimensional systems with coated spheres embedded in a host matrix, and two dimensional systems with coated cylinders embedded in a host matrix.

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MS17
Numerical Methods for Multiscale Kinetic Problems

I will review several recent methods for kinetic problems where the mean free path has different orders of magnitude. In particular, I will present 1) asymptotic-preserving methods: which solve the kinetic problems with numerical resolution at hydrodynamic scales without using the hydrodynamic equations 2) domain decomposition methods: we provide interface conditions that allow us to couple a kinetic equation with a (hydrodynamic) diffusion equation for numerical computation without using iterations at each time step

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MS17
Coarse-Graining and Adaptive Monte Carlo Simulation in Non-Equilibrium Lattice Systems

In recent years there is growing interest in developing coarse-graining methods for atomistic models of complex systems such as polymers, proteins, as well as materials and biological systems. Many of these models rely on parametrized coarse potentials, hence at different conditions (e.g. tempereture, density, composition) need to be reparametrized. Furthermore, since they are not directly derived from the atomistic dynamics it is not clear if they can reproduce transport and dynamic properties. In this talk we present a new mathematical framework for constructing coarse-grained stochastic processes and corresponding coarse-grained Monte Carlo (CGMC) simulations directly from microscopic systems that systematically include subgrid scale information on particle/particle interactions, microscopic dynamics and stochastic fluctuations. Here we discuss as a concrete example of our approach the coarse-graining of microscopic lattice systems and demonstrate analytically and numerically that CGMC methods are capable of describing efficiently much larger scales than conventional lattice Monte Carlo simulations, as well as providing a tool for direct hierarchical modeling across space/time scales. Furthermore, computational comparisons of coarse-grained and microscopic MC simulations along with accompanying rigorous estimates on the loss of information (i.e. relative entropy) between the coarse-grained and the microscopic probability distribution functions (PDF), highlight the regimes where microscopic and CGMC simulations are asymptotically identical. Finally we discuss adaptive Monte Carlo algorithms constructed using the coarse-grained stochastic processes tools we have already developed. The adaptivity criterion is based, in analogy to PDE finite element methods, on a posteriori estimates which in our stochastic context take the form of a posteriori estimations on the loss of information between the coarse-grained and the microscopic PDFs. Aspects of this work is joint with A. J. Majda (Courant), P. Plechac (Warwick) and D.G. Vlachos (Chem. Eng. Delaware).

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MS17
Epitaxial Growth without Slope Selection: Energetics, Coarsening, and Dynamic Scaling

This work concerns a no-slope-selection model for the surface dynamics of epitaxial thin films after roughening transition. The underlying free energy of the film height profile consists of a high-order term that represents the surface diffusion and a lower-order term with negative logarithmic function of gradients that describes a kinetic asymmetry in adatom attachment. A high-order perturbation analysis on such a model reveals nonlinear morphological instabilities that have been observed experimentally. Minimum energy asymptotics and bounds for gradients in the large-system-size limit are derived. Bounds for the interface width, decay of energy, and dynamic scaling are also obtained. This is joint work with J.-G. Liu.

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MS17
Well-Posedness and Simulation of Rod-like Models

Its well-known that the mathematical model of Newtonian fluid is described by Navier-Stokes equations. NS equation is valid for describing the fluid such as the oil, water etc, but for the visco-elastic fluid, such as the egg white, blood and industrial fluid, the linear constitutive relation cant give the right physical phenomena. This kind of fluid is called non-Newtonian fluid or complex fluid. We are interested in the multi-scale physical models of rod-like. In those models, the viscosity is thought of being brought by large amount of polymers in the Newtonian solvent. Each particle of polymers is assumed as a rod. This is a typical two-scale physical problem. In order to describe the motion of the polymers, we use a mesoscopic stochastic differential equation or Smoluchowski equation. The macroscopic fluid equations are still the conservation of mass and momentum, except that an additional term which is given by virtual work principle caused by the polymers contribution. In this talk, we are focused on Doi model. Analyze the well-posedness of the coupled equations (Smoluchowski equation and SDEs) and the convergence of the numerical schemes. We also study the microstructure formation, disclination dynamics and polydomain textures that arise when liquid crystal polymers undergo shear flows.

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MS18
Constructing Partially Regular Solutions for the Generalized Landau-Lifshitz-Gilbert Equations

I will describe some general techniques to construct partially regular weak solution for systems which include the generalized 2-dimensional Landau-Lifshtiz-Gilbert (LLG) equations. While partially regular global weak solutions have been developed for LLG, the existing methods are not constructive. Motivated by the origins of these equations from a discrete system, I consider approximations of systems on a uniform spatial grid. The idea is to show that a sequence of solutions to this approximation converges to a solution to the original equation as the grid-size approaches zero. I will discuss the 2-dimensonal LLG but the techniques developed here can be adapted to to other equations that share the required features as well. My approach rests

on three constructions: (a) the construction of a suitable discretization of LLG; (b) the choice of a frame in which to express the Schrödinger term–which is nonlinear in its highest order term– so that the equations we consider in fact have a linear highest order term; (c) the construction of the discrete fundamental solution of the resulting linear operator and deriving appropriate linear mixed space-time estimates.

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MS18

Interaction Energies for Boundary Vortices in Thin Magnetic Films

We consider the following reduced model for thin film ferromagnetism [Kohn and Slastikov 2003]:

$$E_\varepsilon(m) = \frac{1}{2}\int_\Omega |\nabla m|^2 + \frac{1}{2\varepsilon}\int_{\partial\Omega} (m\cdot n)^2 d\mathcal{H}^\infty$$

in the space $H^1(\Omega, S^1)$, for a simply connected Ω. We show how minimizers develop singularities as $\varepsilon \to 0$, analyze these singularities, and derive a renormalized energy that is determined only by the position of these singularities and the geometry of the domain.

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MS18

Magnetic Switching: pulsed astroids and thermal effects

Pulsed switching experiments study the behavior of small magnetic elements under pulsed applied fields. The zero-temperature astroid is well understood. Remarkably, the experiments recover well-defined "finite temperature astroids." We consider the stochastically perturbed LLG equations under the assumption of spatial uniformity. Applying large deviation theory and prefactor estimates, we derive a mathematical definition of the finite temperature astroid. Contour plots of the probability to switch capture qualitative features of the experimental plots. This work is joint with Robert V. Kohn and Eric Vanden-Eijnden.

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MS18

Another Thin-Film Limit of Micromagnetics

We consider the variational problem of micromagnetics for soft, relatively small thin films with no applied magnetic field. In terms of the film thickness t, the diameter l and the magnetic exchange length w, we study the asymptotic behavior in the small-aspect-ratio limit $t/l \to 0$, when either (a) $w^2/l^2 \gg (t/l)|\log(t/l)|$ or (b) $w^2/l^2 \sim (t/l)|\log(t/l)|$. The limiting variational problem is two-dimensional and local, with no small parameters. The contribution of shape anisotropy reduces, in this limit, to a constant times the boundary integral of $(m\cdot n)^2$.

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MS19

Dynamics of Conformal Maps for a Class of Non-Laplacian Growth Phenomena

For half a century, time-dependent conformal maps have been used to describe continuous Laplacian growth (e.g. viscous fingering), and recently Hastings and Levitov introduced iterated conformal maps for stochastic Laplacian growth (e.g. Diffusion-Limited Aggregation). Here, we extend these methods to non-Laplacian transport processes, such as nonlinear diffusion, advection-diffusion in a potential flow, and electrochemical transport, and simulate fractal growth on curved surfaces and in fluid flows.

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MS19

Conformal Mapping Methods in Viscous Sintering and Related Problems

Viscous sintering is a materials manufacturing process in which a compact of particles is heated so that the particles become mobile, interparticulate-bonds are produced and the particles coalesce as surface energy is released. To model the process macroscopically, it is important to understand the microstructural mechanisms ("unit problems"). This talk will survey recent progress in understanding the mathematics of a simple planar model of this process where the particles are modelled as blobs of very viscous fluid driven by surface tension effects on the fluid boundaries. Conformal mapping methods turn out to play a crucial role, leading to broad classes of exact solutions as well as simple mathematical models. A general discussion of how the mathematical methods used relate to other well-known applications of conformal mapping techniques (e.g. Hele-Shaw flows) will also be presented.

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MS19

Growth of Cylindrical Filaments in Potential Flows

In the paper, potential flows are considered broadly as flows described by its potential. An analysis of the morphological changes of the cross section of growing nuclei is based on the technique of conformal mapping. We discuss the connections of a special non-Laplacian map with some conformal invariants of the flow. Variational principles of conformal mappings augment the linear stability analysis of the growth of a circular nucleus.

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MS19

Conformal Maps, Crossovers and Fixed Points in Diffusion-Limited

Diffusion Limited Aggregation (DLA) is a fundamental stochastic model for describing diffusion-limited growth in the quasistatic regime. The clusters produced are approximately fractal, but a great deal of controversy has been generated by apparent deviations from simple scaling. We show how to use the method of iterated conformal maps to investigate this matter, and to show that there are slow crossovers in DLA which account for the complicated behavior. These corrections to scaling give considerable insight into the structure of the fixed point that governs the asymptotic behavior.

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MS21

Theoretical and Experimental Analysis of Cylindrical Photonic Bandgap Transmission Fibers Across the Infrared Spectrum

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MS21

A Spatial Fourier Transform Technique for the Analysis of General Photonic Crystal Waveguides

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MS21

Mathematical Tools for Quantum Optics of Photonic Crystals

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MS21

Bandgap Cofinement in Photonic Crystal Fibers, Bragg Fibers, and Bragg Onion Resonators

Several numerical methods are presented to illustrate common features in the optical confinement mechanism in photonic crystal fibers, Bragg fibers, and Bragg onion resonators. An intuitive picture is provided to qualitatively explain the main features of loss behaviors of both Bragg fibers and photonic crystal fibers. The novel properties of Bragg onion resonators are also discussed.

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MS22

Network Approximation for Effective Viscosity of Highly Concentrated Random Suspensions

We present a new approach for calculation of effective viscosity of highly packed suspensions of rigid particles in a Newtonian fluid and provide its rigorous mathematical justification. The main idea of this approach is the reduction of the original continuum problem, which is described by PDE with rough coefficients, to a discrete random network. Our mathematical analysis provides an explanation of recent numerical results where the effective viscosity of random suspension of solid particles in a Newtonian fluid was found to be different from earlier predictions based on the lubrication approximation.

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MS22

Elastically Optimal Microstructures in the High-porosity Regime

This talk unifies two themes that have up to now been investigated separately. The first is the analysis of high-porosity microstructures — where attention has mainly been devoted to special structures such as lattices. The second is the design of elastically-optimal microstructures — where a construction known as "sequential lamination" achieves optimality, but not manufacturability, at any value of porosity. We unify these themes by examining a new class of high porosity structures, called "single scale laminates." These structures are simple enough to be easily described and manufactured, yet complex enough to include elastically optimal structures with any (possibly anisotropic) Hooke's law. In 2D, single-scale laminates are

trusses, made using several families of parallel members; the square and triangular lattices are special cases. In 3D they are closed-cell foams, made using several families of parallel thin walls. Mathematically, single-scale laminates can be viewed as sequential laminates "without the separation of scales." We show that in the high-porosity limit, the effective behavior of a single-scale laminate is the same to principal order as that of the associated sequential laminate.

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MS22

Multi-scale Stress Assessment in Composite Structures

Composite structures often sustain nicks or surface damage during service. These provide sources for stress concentration at the boundary of the composite structure. From the perspective of failure initiation it is of practical interest to understand the effect of a boundary stress concentration at the length scale of the microstructure. With this in mind, a new rigorous and systematic multi-scale method for the assessment of the size of over stressed zones inside materials with microstructure is developed. Several examples are provided.

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MS22

Negative Hall coefficients: not the hole story

The Hall coefficient measures the voltage induced across a rectanglar bar when a current flows through the bar and a magnetic field is applied perpendicular to the bar. The electric field generated by the Hall voltage counteracts the force on the moving charge carrier due to the magnetic field. Positive Hall coefficients are usually associated with materials where negatively charged electrons are the predominant carrier, whereas negative Hall coefficients are usually associated with materials, such as doped semiconductors, where positively charged holes are the predominant carrier. However we show here that this is not the complete story. We find it is possible to obtain a material with a negative Hall coefficient by combining materials with positive Hall coefficients in an appropriate microstructure. Also we show it is possible to design microstructures where the effective Hall coefficient is much larger than the coefficient in any of the constituent phases. The situation is reminiscent of similar behavior for the effective thermal expansion coefficient, found by Lakes, Sigmund and Torquato.

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MS23

Time-dependent Solutions to a PDE Model for Superconducting Materials

We present a method for solving the degenerate elliptic-parabolic time-dependent Ginzburg-Landau system describing the order parameter and magnetic potential for a superconducting material in three dimensions in the presence of an applied magnetic field. We obtain classical solutions describing the time-dependent state of the superconductor and find that the vector field of superconducting current in the material is always tangential on the boundary of the domain.

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MS23

Flow Properties of Cholesteric Liquid Crystal Polymers

We develop a model for cholesteric liquid crystal polymers based on tensor theory. A variety of steady structures are obtained. The orientational dynamics in shear flow is investigated.

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MS23

TBA

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MS23

Type I superconductivity near critical temperature

This talk concerns a type I superconductor subjected to an applied magnetic field and slightly below the critical temperature T_c. We use Ginzburg-Landau functional to estimate the value of the critical field H_c, and examine the superconducting behavior when the applied field is below H_c. We also present a result obtained jointly with Yihong Du, which shows that there exists a critical value for the penetration parameter, below which the sample has higher critical field H_c and exhibits a hysteresis phenomenon.

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MS24

Cross-couplings cut through Complexity: Banana Liquid Crystals

Liquid crystal phases (LCs) formed by achiral bent-core molecules (banana LCs) are distinguishable from those of

their classical (i.e. rod/disc-shaped) counterparts with only quadrupolar order. We argue that the interplay between tetrahedratic (octupolar) and quadrupolar order could account for ambidextrous chirality, one of the remarkable features of banana LCs, where left and right-handed chiral domains co-exist.

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MS24

Time Evolution of Nematic Liquid Crystals and Motion by Mean Curvature

We study the asymptotic behavior of the evolution system, modeling the time-dependent behavior of nematic liquid crystals with variable degree of orientation. The system arises from the continuum model of Ericksen in the absence of flow. We establish the appropriate energy law and show the convergence of this system to the version of the mean curvature flow.

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MS24

Antiferroelectric and Ferroelectric Smectic Liquid Crystal Fibers of Bent-core Molecule

Recently the research of ferroelectric liquid crystals of bent-shape molecules revealed delicate chirality and polarity properties. In this talk we will show that these materials also have very unusual rheological features, like formation of stable fluid fibers and bridges. Under electric fields these objects present striking mechanical effects, such as longitudinal and transversal vibrations. The studies indicate that research of banana-liquid crystal fibers may lead to new type of artificial muscle systems.

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MS24

Fast Switching of Electrically Driven Dual Frequency Liquid Crystals

We demonstrate theoretically and experimentally that a dual-frequency nematic liquid crystals can be used to significantly increase the switching speed of electrically-controlled nematic cells. For example, a nematic cell of thickness 15 micrometer can be switched within 0.5 ms instead of the usual 100 ms. The high switching speed is achieved in cells with a high pretilt angle (about 45 degrees) and with frequency and amplitude modulated voltage.

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MS25

Impurity Effects on Grain Boundary Migration: Theory and Computer Simulation

We start from a review of a classical theory for the impurity effect on grain boundary migration. Atomistic computer simulations provide an excellent opportunity to test this theory. We discuss results obtained via kinetic Monte Carlo simulations which show that the key deficiencies of the classical theory are the assumption that the intrinsic and impurity drag effects can be superimposed and not considering the mechanism of grain boundary migration. The last part of the presentation is devoted to a review of recent results obtained via the molecular dynamics simulation of boundary migration in Al in the presence of Fe impurities.

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MS25

Atomic Force Microscopy Study of Grain Boundary Migration

We performed an atomic force microscopy (AFM) study of the areas swept out by grain boundaries that migrated during high temperature annealing of coarse-grained NiAl. We showed that the sharp root of the grain boundary groove formed at original boundary position is smoothening after the beginning of boundary migration process. An analyt-

ical solution for the surface topography in the vicinity of groove root evolving by surface diffusion mechanism was obtained. The comparison of the calculated curvature of the blunted root with the experimentally observed one allowed us to quantify the boundary migration process. In some cases, the grain boundary migration resulted in characteristic ghost line morphology, which is a typical result of jerky, spasmodic migration mode. Quantitative analysis of the topography of ghost line areas allowed us to estimate the time interval between two consecutive jumps of the grain boundary. It was shown that the instantaneous grain boundary velocity can exceed by two orders of magnitude the averaged migration rate estimated according to the migration distance and annealing time. We also analyzed the surface topography in the region of migrated triple junction. The dynamics of grain boundary migration was deduced from the variable dimensions of the grain boundary groove formed at the immobile grain boundary. Taken together, these observations demonstrate a high potential of AFM for post-mortem studies of grain boundary dynamics during high temperature annealings.

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MS25
Mesoscale Issues in Microstructure Simulation

Most technologically useful materials arise as polycrystalline microstructures, composed of a myriad of grains. The orientations and arrangements of the grains are implicated in many material properties across wide scales, for example conductivity, life time, fracture toughness and more. In this talk we discuss multiscale modeling and simulation of grain growth. The starting point is the Mullins equation of growth by mean curvature with the Herring condition at triple junctions. Coarse graining of this model is discussed both in space and time. In particular we focus on a stochastic model in terms of grain area and number of edges is constructed, leading to a master equation which is non-local. Challenges in texture evolution and grain boundary character are discussed.

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MS25
Size Effects during Thermal Evolution of Bulk Nano-Crystalline Microstructures

Recent experimental studies have shown that thermal evolution of nanocrystalline interface microstructures is stable compared to parabolic grain growth observed in coarser microstructures. Here we show that for initial stage growth of these microstructures, the driving force dependence of interface migration rates can no longer be assumed to be linear. We derive the modified growth law due to non-linear interface kinetics, and find that the linear growth observed in experiments is in excellent agreement with sublinear interface kinetics based grain growth predictions. Atomic-scale simulations aimed at understanding the role of additional size dependent kinetics such as grain rotation and triple drag is also presented, and the effect on growth kinetics discussed.

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MS26
Continuum Simulations of Vertically Vibrated Granular Media

We study vertically oscillated granular layers, using molecular dynamics simulations and numerical solutions of continuum equations to Navier-Stokes order. A flat layer of grains is thrown up from an oscillating plate and collides with the plate later in the oscillation cycle, producing shock waves. Molecular dynamics and continuum simulations yield results for the shock position, shape, and speed that agree well. Shock velocity increases continuously with decreasing inelasticity, and the elastic limit is not singular.

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MS26
Shear Inelastic Diluted Flows Modeled by Boltzmann Equations

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MS26
High-Energy Tails for Velocity Distributions in Rapid Granular Flows

Boltzmann-type equations with inelastic interactions appear as kinetic models for rapid flows of granular media. Among many interesting features of solutions of such equations is non-Gaussian behavior of the high-energy tails of velocity distributions. I will present recent work with I. Gamba, A. Bobylev and C. Villani on rigorous derivation of this high-energy behavior. A novel technique for obtaining pointwise estimates for the nonlinear Boltzmann equation, based on a comparison principle, will receive particular attention.

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MS26
Lattice Dynamics and Noise Effects in Patterns in

Oscillated Granular Layers

Vertically oscillated granular layers form standing wave patterns (squares or stripes) when the container acceleration exceeds about 2.5g. We present experiments and molecular dynamnics simulations for the square patterns. As the transition to square patterns is approached, transient disordered waves with a characteristic length scale emerge and increase in power and coherence. The scaling behavior in the vicinity of the transition agrees with the Swift-Hohenberg theory for convection in fluids, but the noise in the granular system is orders of magnitude larger than the thermal noise in a convecting fluid. Above the transition, the square lattice exhibits the normal modes of an atomic lattice. For large mode amplitude, the granular lattice melts. The measured lattice oscillation amplitude at melting is in accord with that the Lindemann criterion for melting in two dimensions. *Work supported by DOE, conducted in collaboration with D. I. Goldman and with M.D. Shattuck, S.J. Moon, and J.B. Swift

Harry Swinney
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Lattice dynamics and noise effects in patterns in

MS27

Scattering Matrix Techniques for Modelling Extended Photonic Crystal Devices

Photonic crystals (PC) will likely amongst be the building blocks of future micro-optical technology, providing the ability to develop integrate all-optical photonic processors. The design of these devices requires the solution of complex coupling/interfacing problem. In this paper, we describe an semi-analytic approach for modelling extended PC devices that is based on the Bloch modes of the device components, present a range of applications and focus on some of the elegant properties that are analytically satisfied by the scattering matrices and the consequent conservation (energy and reciprocity) properties that are satisfied by the modes.

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MS27

Homogenization of Wire Photonic Crystals Leading to Left-Handed Media

We consider a domain of $\mathbf{R}^3$ filled periodically (period η) by parallel rods of radius r and high permittivity ε. We are looking for the asymptotics of the harmonic diffraction problem as the small parameters $\eta, r, \varepsilon^{-1}$ tend to zero. The homogenized medium can possess a magnetic activity, characterized by a permeability $\mu_h(\omega)$. For certain ranges of frequencies μ_h can be negative and the homogenized medium is left-handed if ε is negative as well.

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MS27

Design of Novel Optical

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MS27

Not finalized yet, but highly possible

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MS28

Surface Energies in Non-convex Discrete Systems

The asymptotic study of next-to-nearest neighbor lattice systems as the lattice parameter tends to 0 gives rise to high-order continuum energies with internal and boundary surface energies. We give an analytic description of this phenomenon using Gamma-convergence techniques, highlighting non-local effects.

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MS28

Atomistic and Continuum Models of Solids

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MS28

Mechanical Model of Latent Heating

We consider Hamiltonian dynamics of a bi-stable mass-spring system driven quasi-statically in a hard device. Due to successive flip-over of the individual series elements, the loading beyond instability threshold leads to complex dynamical behavior with intense tunneling of energy from macro to micro-scales. The ensuing equipartition suggests thermodynamic description. For the chain which is initially far from thermal equilibrium we observe a transient phenomenon of irreversible energy conversion into high frequency modes. If the elastic moduli of the energy wells are different, the subsequent quasi-static cycling between phases introduces reversible temperature variations (latent heating) whose magnitude can be predicted by methods of classical statistical mechanics.

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MS28

Coarse-Graining of Atomistic Binding Relations and Universal Macroscopic Cohesive Behavior

We analyze the effective behavior of a large collection of interatomic planes subjected to a prescribed opening displacement at its boundary, with interactions beyond nearest-neighbors and surface relaxation allowed for. The analysis reveals that the macroscopic cohesive law adopts a universal form, independent of material type. Numerical experiments show that the macroscopic cohesive laws of alumninum (a metal), alumina (a ceramic) , and silicon (a semiconductor) indeed collapse to the single universal curve predicted by the theory when properly rescaled.

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MS29

A Description of Strain-driven Formation of Semiconductor Nanostructures

Surface energy plays a central role in the strain–driven formation of semiconductor nanostructures on substrate surfaces. Classical surface diffusion theory predicts symmetry in behavior with respect to the sign of mismatch strain and an energetic barrier to nucleation of perturbations from high symmetry crystallographic orientations, both at variance with observations on SiGe/Si island growth. It is demonstrated that both issues can be resolved by means of a description of surface evolution based on the physics of crystallographically stepped surfaces.

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MS29

Scaling and Coarsening of Step Bunches

Vicinal crystal surfaces driven out of equilibrium by external fluxes often display step bunching instabilities. The shape of a step bunch is determined by the balance between the destabilizing flux and the repulsive step-step interaction. The long-ranged nature of the step-step interaction leads to characteristic scaling laws relating bunch height, bunch width and bunch slope. The talk will introduce discrete step-dynamical models for step bunching induced by growth, sublimation and surface electromigration. In appropriate limits a continuum equation for the surface profile emerges, which allows for a rigorous derivation of the scaling laws and shows that classes of step bunching instabilities follow the same universal behavior. Finally, the question of whether the dynamic coarsening of step bunches can also be described within the continuum theory will be discussed.

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MS29

The Evolution and Self Assembly of Quantum Dots on Surfaces

A major difficulty in realizing the promise of electronic devices using quantum dots is to control the size, shape and location of these nanostructures on surfaces. We find that in stress-free systems wherein the surface of the semiconductor film is unstable to the formation of faceting and in which the film wets the substrate, an instability occurs that can lead to well ordered arrays of dots. The dependence of the island size and location on the nature of the wetting potential and the degree of instability to faceting will be discussed. (Joint work with S. H. Davis, A. A. Golovin, T. Savina)

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MS29

Coarsening Dynamics of Faceted Crystal Surfaces

The morphology and coarsening dynamics of a faceted crystal surface annealed in contact with its melt is known to change dramatically if, in addition, the crystal is subject to net growth. We present a theoretical study of this annealing-to-growth transition by considering representative thermal annealing (A and net-growth (G) continuum models. In each case, our theory provides a complete characterization of the morphology and coarsening dynamics in terms of an associated Edge-Network-Dynamical-System (ENDS). The distinctive coarsening laws $\mathcal{L} \sim \sqcup^{\backslash}$ for the increase in time, t, of the characteristic facet size $\mathcal{L}$, for (A) and (G) follow directly from the scaling properties of the associated ENDS. Large scale numerical simulations of the coarsening dynamics of these edge-networks will also be presented which probe the hypothesis of dynamic scaling and the nature of correlation effects.

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MS30

Electro-mechanical Behavior of Ferroelectric Perovskites

This talk will describe recent theoretical and experimental efforts to understand the electromechanical behavior of ferroelectric perovskites. This work is motivated by the desire to develop an actuator that is suitable for MEMS applications. Domain patterns – i.e., characteristic arrangements of regions with almost uniform electrical polarization – and their evolution is of particular interest.

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MS30

The Phase Transition Between Chiral Nematic and Smectic C* liquid Crystals

We study the Chen-Lubensky model to investigate the phase transition between chiral nematic and smectic C* liquid crystals. First, we prove the existence of the minimizers in an admissible set consisting of order parameters in $H_0^2(\Omega : \mathbf{C})$ and molecular directors in $\mathbf{W}^{1,2}(\Omega : \mathbf{S}^2)$. The splay, twist, and bend Frank constants are considered to be large based on physical observaition. Then we describe the transition temperature when a domain is a considerably large liquid crystal region confined in two plates.

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MS30

Cooperative Effects in a Dye/liquid Crystal System

We discuss the dichroic dye/liquid crystal interaction known as the Janossy effect and studied by Palffy-Muhoray, Kosa and E. A consistent variational principle is offered that takes advantage of Monge-Kanotorovich mass transport ideas and some consequences, like whether or not such a formulation can actually predict the observed Janossy effect, are discussed. This is joint work with Stuart Hastings.

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MS30

Mirrorless Lasing in Liquid Crystalline Bandgap Materials

Due to their periodic structure and birefriengence, certain liquid crystals are self-assembled photonic band-gap materials. Classical wave propagation is forbidden in the stop band, where distributed cavity effects result in photon localization. In optically pumped dye-doped samples, low threshold mirrorless lasing occurs at the band edges; or, due to defects, in mid-band. We present the results of experiments on these materials, and relate these to density of states and coupled mode descriptions.

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MS31

Phase-Field Modelling of Intergranular Films in Silicon Nitride

Amorphous, oxygen rich films with nanometer scale thickness are observed in many ceramics such as silicon carbide, aluminum oxide, and silicon nitride. The goal of this work is to employ a continuum thermo-dynamics based theory to understand the competing effects that stabilize such films. A phase-field model is presented that includes structural, chemical and electrostatic contributions to the free energy. The model is applied to intergranular films in silicon nitride and the results are compared to molecular dynamics and experimental descriptions.

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MS31

Modelling Grain Growth in Crystalline Materials

Polycrystals differ from soap froths in several significant ways; crystalline grains are rigid, their axes are oriented, and properties of their boundaries are anisotropic. Motion and rotation of crystals have been detected and can have significant consequences. Motion of an interface between two crystals can produce a coupled tangential motion of the two crystals relative to each other, and such translations can result in grain rotation during grain growth. We incorporate these effects of crystallinity into postulating a single formulation, and find that several phenomena associated with grain boundary mechanics and motion then follow. The predictions for shrink rates and rotations of circular cylindrical grains moving to reduce total surface free energy are then explored. Among the results we give the conditions for increases in misorientation and surface energy per unit area γ that have been seen in the molecular dynamics

simulations. Another surprising results is that certain conditions, if achievable, can result in increases rather than decreases in radii. A more thorough exploration of a variational model of this formulation with application to noncircular crystals and a variational model will be presented in the companion talk.

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MS31

Modeling of Grain Structure Evolution and Singular Diffusivity

We will present a mathematical model which can reproduce solidification process and grain boundary formation followed by grain structure evolution. The model includes a phase fileld equation coupled with an equation of angle variable which represents orientations of the grains. The key concept of this model is "singular diffusivity" which is derived from the non-differentialble energy functional. It enables us to describe the grain boundary motion and the grain rotation simultaneously. It will be demonstrated how the highly mathematical theory is applied to the modeling in material science.

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MS31

On Growth-Induced Rotation of Embedded Crystals

We apply the principal idea of our companion talk, that normal grain boundary motion should usually be coupled to relative tangential motion of the grains to study shrinking grains of more arbitrary shapes whose rotations would require shape accommodation. A variational model is proposed which includes stress- and capillarity-induced surface diffusion as well as grain growth/shrinkage by attachment-detachment kinetics and grain boundary sliding. When applied in particular to a cylindrical grain of initial shape given in polar coordinates by $R(\rho, 0) = r_o(1 + \epsilon_o \cos(m\rho))$, various conclusions are drawn. In particular, in the no-sliding case the relative rotation of the axes of the crystal lattices is twice that of the rotation of the axes of the grain shape. Furthermore, the anisotropy of the shape might increase rather than decrease under certain conditions.

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MS32

Order-parameter Description of Dense Granular Media

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MS32

A Theory of Cooperative Diffusion in Dense Granular Flows

Many attempts have been made to describe fast, dilute granular flows starting from the kinetic theory of gases, but slow, dense flows require a fundamentally different approach, due to long-lasting, many-body contacts. In the case of slow drainage, various continuum models have been proposed for the mean flow, but no microscopic theory of fluctuations is available. Here, a new model is proposed which postulates that particles undergo cooperative random motion in response to diffusing "spots" of free volume. The Spot Model may be used in discrete simulations or analyzed in the continuum limit, where some new partial differential equations arise. It predicts spatial velocity correlations, slow cage breaking, and geometry-dominated diffusion in good agreement with particle-tracking experiments in our laboratory.

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MS32

Dense Granular Flows

Non-thermal yet disordered, strongly dissipative yet rigid, the mechanics of packings of grains has fascinated physicists and engineers at least since the time of Coulomb. This talk will focus on one of the classical problems in this field, the behavior of dense granular flows driven by gravity. I will give examples of such flows drawn from geophysics, and then introduce some of the ideas of Ralph Bagnold, who developed the concepts on which the modern study of granular flows are based. A systematic phenomenology of dense granular flows down inclines has recently been developed, based both on numerical work and on experiments. This phenomenology emphasizes the role of inelastic collapse in controlling the rheology of these flows, and hints at the structure of an ultimate theory of dense flows.

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MS32

Molecular Dynamics Simulations of Dense Granu-

lar Hopper Flows

Large-scale three dimensional molecular dynamics simulations of hopper flow are presented. The changes in internal structure and force distributions with decreasing flow velocity are described in depth. Hopper flow has recently been suggested by many groups as an ideal system for studying the onset of jamming, both experimentally and through simulations. While changing flow velocities as the system approaches jamming have only a small effect on the force distribution, they have a large effect on the impulse distribution. These macroscopic distributions are related to the dynamics of individual particles in the flow.

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MS33

Nonlinear Maxwell Equations in Inhomogeneous Media

We study the basic properties of the Maxwell equations for nonlinear inhomogeneous media. Assuming the classical nonlinear optics representation for the nonlinear polarization as a power series, we show that the solution exists and is unique in an appropriate space if the excitation current is not too large. The solution to the nonlinear Maxwell equations is represented as a power series in terms of the solution of the corresponding linear Maxwell equations. This representation holds at least for the time period inversely proportional to the appropriate norm of the solution to the linear Maxwell equation. We derive recursive formulas for the terms of the power series for the solution including an explicit formula for the first significant term attributed to the nonlinearity. The developed approach allows, in particular, to rigorously derive the Nonlinear Schrodinger equation as an approximation to the relevant Nonlinear Maxwell equation, and provides estimates on the accuracy of the approximation.

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MS33

On Spectra of "Soft Wall" Waveguides

The talk is devoted to some problems of spectral theory of waveguides that allow evansecent waves to escape rather than confining them with boundary value conditions. Examples include linear defects in photonic band gap structures and Schroedinger operators with a delta type potential supported by a curve.

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MS33

Anomalous Transmission in the Presence of Guided Modes

The interaction of electromagnetic source fields with guided modes in periodic slabs causes resonant scattering behavior. It has been observed experimentally and by numerical methods that this resonance is associated with sharp peaks and dips in the transmission coefficient. We explain the resonant scattering and transmission anomalies by means of an analytic theory of the fields as functions of frequency and Bloch wave number.

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MS33

Resonances and Bound States in Periodic Slab Structures

We study resonant fields in periodic slab structures known in the physics and engineering literature as "leaky modes" or "quasi-guided modes". We formulate a precise mathematical theory for such fields by using analyticity to extend the notions of radiation condition and source to complex frequency and Bloch wavenumber. We are able to explain analytically resonant phenomena that have been observed in physical and numerical experiments.

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MS34

A Random Weak Membrane Model

Blake-Zisserman weak membrane is a finite-difference model whose continuous counterpart is an anisotropic Mumford-Shah energy. We propose a random version where the 'weak connections' are randomly mixed with quadratic ones; the corresponding Gamma-limits are related with results in percolation theory.

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MS34

Nematic Elatomers: A Case Study on Quasiconvex Envelopes Coming from Materials Science

Relaxation techniques for non quasiconvex energies have been been usually motivated by the attempts to characterize the macroscopic response of crystalline solids. We show how extending the scope of attention to amorphous materials (in particular, polymeric gels) may lead to results of unprecedented sharpness.

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MS34

Regularity Results for Nonconvex Variational Problems

We consider regularity questions for nonconvex variational problems related to mathematical models for solids undergoing solid to solid phase transformations. The methods are purely variational and can be applied to classical solutions as well as to generalized solutions (minimizing Young measures). This is joint work with J. Kristensen and K. Zhang.

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MS34

Single-slip Elastoplastic Microstructures

We consider rate-independent crystal plasticity with constrained elasticity and state the variational formulation of the incremental problem. For generic boundary data, even the first time-increment does not admit a smooth solution and fine structures are formed. Solutions with microstructures are constructed by forming laminates between two different deformation gradients. For the concrete case of a simple shear test it can be shown that these generalised time-discrete solutions converge to solution of the time continuous evolution problem.

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MS35

Modeling iron at the *bcc–hcp* phase boundary

The measured *bcc*–to–*hcp* transformation pressures in iron display variability between experiments, where these experiments suggest an approximate value of 13 GPa. To investigate this transformation we have developed a multiscale iron model that contains a first–principles based energy function, which depends on the energetics of *bcc* and *hcp* phases, the *bcc* to *hcp* transformation path, and the construction of a kinematically compatible mixture of phases. This iron model proves to be quite sensitive to shear stresses, where the inclusion or omission of these stresses cause the transformation pressure to vary significantly. Additionally, the *hcp*–to–*bcc* transformation occurs at a pressure much lower than the *bcc*–to–*hcp* transformation, resulting in a hysteresis width of ≈5 GPa due to kinematics rather than kinetics.

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MS35

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MS35

Coarsening in stochastically perturbed Ginzburg-Landau gradient flows

We demonstrate how the stochastic Allen-Cahn equation in one spatial dimension can be reduced to an ensemble of Brownian walkers mutually annihilating at collision. The technique is also applied to other stochastically perturbed gradient flows for the Ginzburg-Landau functional, e. g., generated by the constrained Allen-Cahn and Cahn-Hilliard equations, where the similar results are obtained.

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MS35

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MS36

Magnetic Tiles - A New Perspective on Ferromagnetic Shape Memory Alloys

This work will discuss the temperature and field dependent

evolution of the micromagnetic structure in ferromagnetic shape memory alloys (Ni-Mn-Ga and Fe-Pd). Results provide a new and simple perspective on these actuator materials - the micromagnetic structure of these alloys truly resembles a magnetic 'mosaic' contained within 'tiles' of the transformed martensite phase (twins). These results also answer the fundamental question, viz., what is the nature of the magneto-elastic coupling in these alloys and to what extent does it drive structural transformation? It is shown that the temperature dependent reconfiguration of the micromagnetic structure is completely enslaved to and follows the martensitic transformation in these alloys. Direct micromagnetic evidence of field induced martensitic transformation is also shown. This field induced martensite transformation was found to be completely reversible. In analogy with the well known pseudo-elastic behavior in conventional shape memory alloys, this behavior is termed 'magneto-pseudo-elastic' or MPE effect. Remarkably, the MPE effect can be realized in fields (800 Oe) that are much lower than theoretically predicted values of several thousand oersteds. Finally, the concept of magnetic mosaics has been used to synthesize a novel class of materials with engineered magnetic anisotropies, and will be discussed. This work was supported by the DOE, Office of Basic Energy Science, Grant No. DE-FG02-01ER45906, and this support is gratefully acknowledged. Contact Address: Professor Harsh Deep Chopra, Mechanical and Aerospace Engineering Department, 613 Furnas Hall, State University of New York at Buffalo, Buffalo, NY 14260, USA. E-mail: hchopra@eng.buffalo.edu

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MS36

Magnetization Reversal and Hysteresis in Nanocrystalline Ferromagnets

In this talk, we report an effective medium theory on magnetization reversal and hysteresis in the magnetically interacting nanoparticles, where the inter-granular magneto-static interaction is accounted for by an effective medium approximation. We consider an assemblage of single-phase single-domain magnetic particles, with particle size smaller than the single domain limit so that no domain wall movement is involved, yet large enough compared to the exchange length so that the short-range exchange coupling can be ignored. Two dimensionless parameters λ and h_0 are introduced, which completely characterize the hysteresis of ferromagnetic polycrystal. The competition between the anisotropy energy and the inter-granular magneto-static energy is measured by λ, while the competition between the anisotropy energy and Zeeman's energy is measured by h_0. The hysteresis loop, magneto-static energy density, and anisotropy energy density calculated using this theory agrees well with micromagnetic simulations. The calculations also reveal that the sub-nucleation field switching due to the magnetic field fluctuation is important when the magnet is not very hard, and a energy surface based probability model has been developed to address that.

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MS36

Ferromagnetic shape memory composites

Ferromagnetic shape memory (FSM) composites can be made by embedding fine FSM particles in a much softer polymer matrix. Under the application of external magnetic field and mechanical load, the FSM particles undergo a macroscopic deformation, which induces an overall deformation of the composite. We present theoretical models to predict the effective properties of a ferromagnetic composite, in both the low volume fraction limit and for higher volume fractions. We assume the FSM particles obey constrained theory, such that the strain of the particles arise only from variant motion; no superposed elastic strain or rotation of the magnetization is allowed. We also consider the elastic energy of the surrounding matrix owing to particle deformation. In the low volume fraction limit, the particle energy and the elastic energy can be computed explicitly for elliposidal particles, using micromagnetics and a variation of Eshelby's method. This leads to a quadratic programming problem for the effective properties of the composite. For higher volume fractions, where interactions among FSM particles are important, we use two-scale convergence methods to obtain a variational principle for the properties of the composite. Results are presented for both Ni_2MnGa and $Tb_xDy_{(1-x)}Fe$ composites.

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MS36

Modeling magnetic-field-induced strain in Ni-Mn-Ga

The topic of Ferromagnetic Shape-Memory alloys has received a lot of attention from the scientific community since the unusually large magnetic field-induced strain of Ni-Mn-Ga was demonstrated in 1996 by Ullakko and colleagues. To date, a record 9.7% magnetic field-induced strain has been obtained in Ni-Mn-Ga single crystals, up to frequencies of the order of a Hz, for example by M llner et al. (2004). It is of great interest for the applications' design, as well as the material's enhancement to accurately model the actuation mechanism in these materials. Early models have focused on the macroscopic response of Ni-Mn-Ga single crystals to an applied field and stress, with reasonable experimental agreement. These models succeeded in relating the general shape of the strain output to the static stresses and magnetic fields. With subsequent studies of the dynamic properties of Ni-Mn-Ga , microscopic modeling became a necessity, and was recently addressed by Paul and others. Other directions in which research has been moving are the effects of acoustic stress waves, such as those applied with a piezo-electric stack, on field-induced strain. Finally, the study of polymer-FSMA composites has shown the need for estimates of the polycrystalline response and its texture dependence, a matter that has been addressed by Marioni et al. and in a more general way foe example by Bhattacharya, in relation to the conventional shape-memory effect. This talk aims at presenting

an overview of parts of the work that has been done in the aforementioned areas, as well as challenges that have not yet been answered.

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MS37

Coarsening Processes in Homoepitaxial Thin Films: Atomistic and Continuum Modeling

Homoepitaxial deposition processes create distributions of adsorbed 2D islands or clusters, which subsequently coarsen. Coarsening often occurs via Smoluchowski ripening, i.e., via cluster diffusion and coalescence [Wen et al., PRL 76, 652 (1996)] rather than via Ostwald ripening. Experiments often reveal transient behavior reflecting the "initial" conditions determined by the deposition process, not simple temporal scaling predicted by asymptotic theories. After some review, we focus on atomistic and continuum modeling of cluster diffusion and coalescence, specifically size-scaling and the limitations of continuum modeling on the nanoscale [Liu and Evans, PRB 66, 165407 (2002)].

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MS37

On the Effect of Screening and Correlation in Domain Coarsening

The classical theory by Lifshitz, Slyozov and Wagner describes diffusion limited coarsening of particles in the limit of vanishing volume fraction ϕ. Due to several shortcomings of the LSW theory there is a large interest in deriving first order corrections which take finite volume fraction effects into account. We discuss a new method to effeciently identify first-order corrections in a statistically homogeneous system. The key idea is to relate the full system of particles to systems where a finite number of particles has been removed. This method allows to decouple screening and correlation effects and allows to effiently evaluate conditional expected values of the particle growth rates.

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MS37

Long-time Asymptotics of the LSW Model

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MS37

Upper Bounds on Coarsening Rates for an Epitaxial Growth Model

Coarsening phenomena have been observed in many energy driven models from materials science. A lot of work has been done in physics and numerics exploring the coarsening exponent for various models. However, rigorous analysis is still lacking. In this talk, we prove a rigorous upper bound on coarsening rate for isotropic epitaxial growth model. At this stage, we can only prove a weak version on the upper bound. The proof essentially follow a framework introduced by Kohn and Otto in study of phase ordering. Proof also relies on compactness results for Aviles-Giga energy. This is joint work with R. V. Kohn.

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MS38

The Mystery of Booming Sand Dunes

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MS38

Effective Temperature in Dense Granular Systems

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MS38

Equation-Free Coarse-Grained Analysis of Granular Flows

Systematic derivation of continuum equations for realistic granular flows, beyond smooth inelastic hard spheres in vacuum, is a difficult task, because they often violate basic assumptions in the mean-field kinetic theory. However, microscopic models such as molecular dynamics simulation accurately describe most of complicated granular flows, which have been extensively used to enhance our understanding on granular flows. In this talk, we will demonstrate how the recently developed "equation-free multiscale computational method" [Theodoropoulos *et al.*, PNAS, **97**, 9840 (2000)] can be wrapped around the molecular dynamics simulation to study coarse-grained continuum-level dynamics of granular flows, without attempting to derive continuum equations.

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MS38

Two-dimensional Equilibria Related to Steady Granular Flow in a Conical Hopper

The full equations of granular flow in a converging hopper are thought to be reliable enough for industrial design. However, they suffer from two main mathematical difficulties. First, the system is hyperbolic, so that the issue of appropriate boundary conditions (where to pose stress and velocity boundary conditions) is problematic. Second, the time-dependent system is ill-posed. In this talk, I address these two issues, along with lesser concerns such as transitions between active and passive stresses, in the context of antiplane shear, leading to a much simpler system that nonetheless retains the mathematical difficulties. One interesting feature of numerical simulations is that the spatially discretized system exhibits fluctuations limited by nonlinearity; the long-time behavior that emerges exhibits some of the structure of the underlying equilibrium of the steady equations.

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MS39

Photonic Waveguide of Coupled Microcavities with Whispering Gallery Modes

In this talk, we will present the results on a study of the optical coupling by evanescent whispering gallery modes between microcylinders, the building blocks of Coupled Resonator Optical Waveguide (CROW) devices. Such waveguides have applications in optical buffering and delay lines in controlling the speed of light propagations. We first construct a high order discontinuous spectral element method using Dubiner orthogonal basis on triangles and Legendre nodal orthogonal basis over quadrilaterals. After validating the exponential convergence of the numerical method, we conduct a systematic study of the optical energy coupling between two microcylinders and demonstrate the successful coupling between the microcylinders and also the dependence of such a coupling on the separation and size deviation of the microcylinders.

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MS39

A new boundary integral equation method for photonic crystal devices

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MS39

Optimal Design of Photonic Crystals

Designing photonic crystal structures with desired properties is difficult. Light behavior inside photonic crystals can be sensitive to geometry and other problem parameters, and is sometimes counterintuitive. However for given design objectives, it is often possible to formulate well-posed mathematical problems, the solutions of which yield structures with the desired properties. This talk is an overview of several such optimal design problems involving photonic crystals, including maximization of band gaps, and maximization of energy density in a point defect mode. A fundamental feature of these problems is that we seek complete device geometries, rather than just several parameters in predetermined geometrical configurations.

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MS39

High-order Fourier/Chebyshev Methods for Large Eigenvalue Problems of Photonics

Analysis of wave propagation in photonic crystals and optical fibers requires accurate numerical solution of large-scale eigenvalue problems. High accuracy needed for modern engineering applicaions is difficult to achieve by traditional methods. We thus present a novel approach to the design of fast, high order eigensolvers. Efficiency and spectral accuracy is achieved by the use of (i) partitions of unity, (ii) structured overlapping grids confirming to the material interfaces, (iii) Chebyshev and Fourier spectral algorithms on the computational subdomains, and (iv) fast high-order interpolation between the subdomains. Our preliminary numerical results confirm that such numerical approach indeed leads to highly accurate and efficient computations.

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MS40
Existence Results for Variational Models in Fracture Mechanics

The talk will present some recent existence results for the variational model of crack growth in brittle materials proposed by Francfort and Marigo in 1998. These results, obtained in collaboration with Francfort and Toader, deal with the n-dimensional case, with a quasiconvex bulk energy and with prescribed boundary deformations and applied loads, both depending on time.

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MS40
A Variational Formulation for the Dislocations on Crystals

Various type of approaches have been proposed in order to model the energy of dislocations and to describe their formation. We propose a variational model based on the Nabarro-Peierls approach. It describes the dislocations by means of a phase field minimizing a non local phase transition type energy.

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MS40
Renormalized Energy and Forces on Dislocations

We present a variational formulation of the equilibrium problem for a finite number of dislocations in a plane domain, and characterize the energy content of a body with isolated defects in terms of a regular function of the defect configuration, the renormalized energy.

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MS40
Cross-Tie Patterns in Micromagnetics-Type Phase Transition Models

We discuss Gamma-convergence for some phase transition type models originating in micromagnetics, prove optimal estimates and exhibit optimal two dimensional transition profiles.

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MS41
Nonlinear Elasticity of Carbon Nanotubes from Atomistic Models

Starting from a disctete model for carbon nanotubes, a method is proposed to systematically construct a hyperelastic material model for a two-dimensional continuum. This method relies on crystal elasticity ideas (the Cauchy-Born rule), which must be extended to deal with a curved 2D lattice deforming in 3D. The extension is inspired in the geometry of the deformation. The surface model accurately mimics the parent discrete model in the full nonlinear regime.

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MS41
Massively Parallel Dislocation Dynamics and Crystal Plasticity

Prediction of the plastic strength of single crystals based on the collective dynamics of dislocations has been a grand challenge for computational materials science for a number of years. The difficulty lies in the inability of the available dislocation dynamics (DD) codes to handle a sufficiently large number of dislocation lines, in order to be statistically representative and to reproduce experimentally observed microstructures. Our new massively parallel DD code is capable of modeling million dislocations simultaneously by employing thousands of processors. We will discuss the methods that make simulations of such scale possible. Simulation data on strain hardening and spontaneous dislocation patterning in FCC and BCC metals will be presented and compared with experiments. We will discuss what sort of new information can be extracted from such simulations and examine how close we are able to come to understanding single crystal plasticity from the underlying collective motion of dislocations. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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MS42
Energy-minimizing microstructures in multiphase elastic solids

This talk concerns problems of microstructure and its macroscopic consequences in multiphase elastic solids, both single crystals and polycrystals. We compute the relaxation under fixed volume fraction for a two-well linearized elastic energy in two and three dimensions with no restrictions on the elastic moduli and transformation strains; and show that there always exist rank-I, -II or -III laminates that are extremal. By minimizing over the volume fraction we obtain the quasiconvex envelope of the energy. We relate these results to experimental observations on the equilibrium morphology and behavior under external loads of precipitates in Nickel superalloys. Predicting the recoverable strains of shape memory polycrystals is a central open problem in the study of shape memory alloys. Our contributions to the solution of this problem are twofold: We show that stress fields in shape memory polycrystals could be concentrated on lower-dimensional surfaces. We do this by proving a dual variational characterization of the recoverable strains of shape memory polycrystals and presenting several examples. Implications of this characterization for effective properties and the development of numerical methods are discussed. We also show that for polycrystals made of materials undergoing cubic-tetragonal transformations the strains fields associated with macroscopic recoverable strains are related to the solutions of hyperbolic partial differential equations. We explore consequences of this relationship and connections to previous conjectures characterizing those polycrystals with non-trivial recoverable strain.

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MS42
Experimentally-Based Mathematical Modeling of the Nano-Scale Mechanisms of Actuation of Ionic Polymer Metal Composites

Ionic polymer-metal composites (IPMCs) are soft actuators and sensors. They generally consist of a thin polyelectrolyte membrane of Nafion, Flemion, or Aciplex, plated on both faces by a noble metal, generally platinum or gold or platinum with a layer of finishing fold to improve surface conductivity, and is neutralized with the necessary amount of counter-ions, balancing the charge of anions covalently fixed to the backbone membrane. The anions in Aciples and Nafion are sulfonates, whereas those in Flemion are carboxylates. When a thin strip of an IPMC membrane in the hydrated state is stimulated by the application of a small (1 to 3 V) alternating potential, it undergoes a bending vibration at the frequency of the applied voltage, generally no more than a few tens of Hertz. Under a suddenly applied step voltage (direct current, DC), the composite quickly bends towards the anode. For the Nafion-based IPMCs that are neutralized with metallic cations, the strip then slowly relaxes in the opposite direction, i.e., towards the cathnode, while still under the applied voltage. The extent of this back relaxation depends on the level of hydration and the cation form. For certain cations, e.g., Cs+ and particularly T1+, the back relaxation is several times greater than the initial fast displacement. If the two faces of this strip are then suddenly shorted, the strip quickly bends further towards the cathode and then slowly relaxes back towards the anode, seldom attaining its original state. The magnitude and speed of these deflections depend on the nature of the counter-ions, the structure of the electrodes, the level of hydration (solvent saturation), and other conditions. When the same membrane is suddenly bent, a small voltage of the other millivolts is produced across its faces. Hence, these IPMCs are soft actuators and sensors. Based on a series of experimental characterizations of the electro-chemo-mechanical properties of bare ionomers and the corresponding IPMCs, various nano-scale mechanisms responsible for the basic properties and the actuation/sensing of IPMCs are mathematically modeled and the results are compared with experimental observations. The mathematical modeling includes analytic solution of the coupled chemo-electric and elastic equations. This is supplemented by numerical solutions and direct comparison with experiments.

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MS42
Formation and Motion of Phase Boundary in Nano-Grained Polycrystalline

Helical-type martensite band nucleation and propagation in superelastic NiTi SMA microtube under uniaxial tension and tension/torsion has been observed recently. This talk reports and discusses this phenomenon from continuum mechanics point of view. Preliminary progress of the investigation on such pattern-forming deformation instability process during stress-induced phase transformation is summarized as follows. (1) Based on detailed experimental observation and possible deformation mechanism, a simple trilinear stress-strain relation with intrinsic strain softening is proposed to approximate the material constitutive behavior during stress-induced transformation. (2) Three-dimensional finite deformation simulation of the tube under loading was performed to model the detailed band nucleation and growth process. A combined analytical-experimental approach is used to extract the constitutive parameters of the material from the experimental measure-

ment. The observed phase boundary motion and deformation patterns are successfully reproduced in the simulation by the identified trilinear constitutive law. The results demonstrated that only geometry instability due to finite deformation is not sufficient to quantify the experimental observation, both material and geometric instabilities, as well as the competition between bulk and surface energy play important roles in the observed martensite band morphology and its evolution. (3) Compared with the investigations based on a similar local constitutive theory, the issue of mesh sensitivity in the nucleation process of the martensite is addressed and demonstrated in the present simulation in the tube geometry. This important issue indicated that interfacial energy must be taken into consideration, which needs to be quantified by a nonlocal model in the future investigation. Finally some difficult issues in building theoretical model for transforming polycrystals are discussed. Acknowledgements - This work has been supported by the Research Grants Council of the Hong Kong Special Administrative Region, China (Project No. HKUST 6074/00E and HKUST 6234/01E) and the Hong Kong University of Sci. & Tech. (Project No. HIA01/02.EG18).

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MS42

High Dielectric Constant Polymer Composites - Effect of the Morphology and Physical Properties of the Constituents

This talk discusses progress made recently in my group to address the issue of how to raise the dielectric constant of polymeric materials substantially above the current level which is relatively low (about 10) in comparison with inorganic materials ($> 1,000$). Polymeric materials with high dielectric constant are attracted for a broad range of applications, including high efficiency charge storage devices and electromechanical devices. Making use of the percolation phenomenon, we demonstrated that in a conductive polymer composites, an all-polymer blend can reach a dielectric constant of more than 2,000. As a result, a strain of 2.7% can be induced under a field of 16 MV/m, which is a substantial reduction in the applied field compared with other electroactive polymers. Furthermore, a three component composite was also investigated, which combines the dielectric- and percolative-composite approach. In this three-component composite, a high dielectric constant organic particulate enhances the dielectric constant of the polymer matrix and this combined two-component dielectric matrix in turn serves as the high dielectric constant host for the conductive polymer to realize percolative phenomenon and further enhance dielectric response. As a result, even with 14 vol% of conductive polymer fillers in the composite, the three-component composites can reach an enhanced dielectric constant of more than 100 times that of the polymer matrix. Moreover, the all-organic electroactive composite actuator material with high electromechanical response, i.e., a 9.3 % strain with an elastic energy density of 0.4 J/cm3 induced under an electric field of 20 V/mm, has been demonstrated. In this talk, we will also analyze the influence of the high dielectric constant filler arrangement in the polymer matrix on the composite and blend dielectric constant. It will be shown that the dielectric response is very sensitive to the arrangement, the shape, size of the fillers in the matrix and a very high dielectric constant can be reached in a composite with certain special filler arrangements.

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MS43

Asymptotics and coarsening in grain growth models

We study dynamics of continuum grain growth models in the asympotic limit of thin boundaries and derive reduced equations governing evolution of the domain walls. We further analyse these equations and construct a toy model which captures the major statistical features of the original dynamics.

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MS43

Coarsening of Fluid Films

Dewetting processes of thin fluid films lead to pattern formation and eventual coarsening. The late stage behavior can be derived through formal asymptotic methods, showing two behaviors: mass exchange and drift. This gives rise to a rich set of dynamics which include both collapse and coalescence of liquid droplets. Scale invariance and power-law behavior of long-term coarsening is explained.

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MS43

Evolution of Pattern Complexity in Cahn-Hilliard Models

Phase separation processes in binary alloys can produce intriguing and complicated patterns. Yet, characterizing the geometry of these patterns quantitatively can be quite challenging. In this talk I will employ computational algebraic topology methods to obtain such a characterization for the complex microstructures observed during spinodal

decomposition and early coarsening in both deterministic and stochastic Cahn-Hilliard models. While these models produce evolving patterns which seem to be qualitatively similar, the topological characterization uncovers significant differences.

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MS43

Coarsening Dynamics in a Model of Shear Bands

We study a finite-difference discretization of an ill-posed nonlinear parabolic partial differential equation. The PDE is the one-dimensional version of a model for the formation of shear bands via anti-plane shear of a granular medium. We derive analytically, and observed numerically, a two-stage evolution leading to a steady-state: (i) an initial growth of grid-scale instabilities, and (ii) coarsening dynamics. In the coarsening phase, one shear band after another collapses until a steady-state with just one jump discontinuity is achieved. Analyzing data from the simulations, we observe that the number of shear bands at time t decays like $t^{-1/3}$. From this scaling law we show that the time-scale of the coarsening phase in the evolution of this model for granular media critically depends on the discreteness of the model.

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MS44

The Inelastic Maxwell Model

Velocity Statistics of inelastic gases are analyzed within the Maxwell Model framework, a kinetic theory with a velocity independent collision rate. In the unforced case, the velocity distributions are self-similar and have algebraic tails with continuously varying exponents. As a result, the velocity moments exhibit multiscaling. In the forced case, the velocity distributions have an exponential high-energy tail (as well as a Maxwellian core if the inelasticity degree is small). The relevance to experiments and the relation between the similarity solutions and traveling waves are also discussed.

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MS45

Complete Transmission Through a Two-Dimensional Diffraction Grating

The propagation of a normally incident plane electromagnetic wave through a two-dimensional metallic grating, will be modeled and analyzed. The period of the structure A is on the order of the incident wave length, but the height of the channel H separating the blocks is very small. Exploiting the small parameter H/A we will develop an approximate transmission coefficient for the grating. For a fixed frequency we shall demonstrate that this coefficient is O(H/A) except near resonant lengths where it is O(1). That is, for certain widths the structure is transparent. Similarly, for a fixed length we shall show that the transmission coefficient has the same resonant features as a function of frequency. This feature makes the grating useful as an element of an optical filter, i.e., only electromagnetic waves with very select frequencies pass through it. On the other hand, the grating possesses broad stop bands in which the structure is opaque. This feature makes the grating a possible component in an optical Fabry-Perot resonator.

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MS45

Transmission of Electromagnetic Waves through Single and Periodically Structured Subwavelength Apertures

Below the plasma frequency, the dielectric response of metals is governed by a negative dielectric function. Associated to this fact is the appearance of surface electomagnetic modes. In this talk we address, from the theoretical point of view, two recently discovered physical phenomena associated to the excitation of these resonances: i) extraordinary optical transmission through single and periodically structured subwavelength apertures and ii) beaming of light through single apertures surrounded by periodic corrugations.

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MS45

Effective Fields and Nonlinear Optical Propagation in Artificially Structured Materials

Approximate equations for nonlinear optical propagation, such as the nonlinear Schroedinger equation and the nonlinear coupled mode equations, have been very powerful tools in elucidating the nature of nonlinear wave propagation, even when detailed studies have implemented full numerical solutions. Recently we have modified the usual multiple scales route to such equations, so as to base their derivation a Hamiltonian formulation of fundamental equations, using a new set of effective fields. This allows for the physical understanding of conserved quantities result-

ing from symmetries in the approximate equations, and permits an easy quantization of the theory. We review the application of this approach to the study of nonlinear propagation and mixing in photonic crystals, and then present recent work in which it is applied to a more general set of artificially structured materials. Of particular interest is a sequence of coupled microresonators, which should allow for nonlinear optical propagation and switching effects at much lower intensities than in more usual structures.

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MS45

Waveguide-plasmon Polaritons in Photonic Crystal Slabs with Metal Ranowires

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MS46

Can Triple Junction Energy Contribute to the Driving Force for Grain Growth?

We discuss the requirements for reliable measurements of triple junction energy and present an experimental estimate of its magnitude in gold. We consider the characteristics of grain growth under conditions where triple junction energy is significant but grain boundary energy is negligible, and show that the behavior differs in many respects from the grain growth model of Von Neumann and Mullins.

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MS46

A Reduced Model for Two-dimensional Grain Growth

We study a model for two–dimensional grain growth, with the aim to capture the long-time statistics of large systems. This model relies on the gradient flow structure of the mean curvature flow which is restricted to straight grain boundaries. We show results of numerical simulations and also study the influence of certain anisotropic surface energies.

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MS46

Abnormal Grain Growth and the Potts Model

Abnormal grain growth is a microscopists' term for the development of a bimodal distribution of domain sizes during a coarsening process. In engineering materials, such behavior is both useful and a nuisance, depending on the circumstances. Some simple ideas are presented for predicting the development of abnormal grain growth as a function of the mobility and energy of the constituent boundaries. These are then compared to the behavior of a multi-state Ising (Potts) model. For the particular example of domain coarsening in a subgrain structure (all boundaries possessing low angle grain boundary character), the agreement is good.

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MS46

Boundary Tracking Simulation of Anisotropic Grain Growth and Grain Boundary Statistics

It is generally believed that grain boundary (GB) statistics are more informative than grain size statistics on GB properties, such as GB energy and mobility. In this talk, I will present some work aimed at characterizing GB statistics in 2D boundary tracking computer simulations of grain growth with anisotropic GB energy and mobility. The mathematical theory and numerical implementation of the boundary tracking simulation are first reviewed. Simulation results with various fictitious forms of GB energy are then presented. It is surprising that whether one postulates that GB energy depends on GB orientation has a dramatic effect on whether one can fit the resulting statistics by a simple Gibbs formula. As a preliminary attempt to explain this, a colored-noise model for GB statistics will be presented in the end of the talk.

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MS47

Mixed continuum/atomistic analysis of nanovoid cavitation

Growth and coalescence of nanosized voids are primary mechanisms of ductile fracture and spallation in metals. We wish to report results of nanovoid expansion (cavitation) in Al and Fe, with special emphasis on the mechanisms operative at the onset of plastic deformation and on the ensuing unconfined plastic flow. The quasicontinuum method is used in order to study realistic-size samples and effectively isolate the voids from spurious image effects introduced by the computational boundary. In order to track large quantities of dislocations effectively, we couple the quasicontinuum region to a model of dislocation dynamics at the far field. The main outcomes of the analysis are the elucidation of the different deformation regimes attendant to nanovoid cavitation and the dislocation structures underlying the regimes; and the macroscopic pressure-volume response of a control volume of the material containing one nanovoid.

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MS47
Thermal Fluctuations on Large Domains

Large deviation theory explains the switching mechanism of systems on finite domains. On sufficiently large domains, however, this picture breaks down. We consider the effect of small thermal fluctuations via

$$u_t = u_{xx} - V'(u) + \sqrt{\epsilon}\eta$$

where η is a space-time white noise and V is an asymmetric potential. Applying large deviation theory and prefactor estimates on appropriately scaled *subcells*, we derive a reduced model which consists of Poisson-distributed nucleation events and deterministic wall propagation. This work is joint with Robert V. Kohn, Felix Otto, and Eric Vanden-Eijnden.

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MS47
TBA - Rudd

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MS47
Coupling Kinetic Monte-Carlo and Continuum Models

We present a hybrid scheme for simulating epitaxial growth that combines the Burton-Cabrera-Frank (BCF) model with kinetic Monte-Carlo (KMC) simulation. This is the first implementation of the scheme for "2+1" dimensional growth. Other improvements over an earlier version include the use of a more conventional KMC model and some refinement in the handling of the boundary condition between the KMC and continuum regions. The method is used to examine unstable step-flow with direct comparison to KMC simulations. The results are extremely good with respect to computational speed and reveal effects due to fluctuations to a much greater extent than the BCF model alone. This method will be especially useful in scenarios with widely separated steps and high adatom densities, as these are situations that cannot be easily simulated with KMC due to increased computational cost. The hybrid method is extremely flexible and can be coupled interchangeably to any KMC scheme.

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MS47
TBA - Vanden-Eijnden

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MS48
Discrete traveling waves: Defects in crystals

The study of dislocations in cristalline solids involves phenomena taking place at different interacting scales: from the nanoscale (a few atomic spacings, the width of dislocation cores) to the macroscale, where the collective behavior of dislocation densities controls properties such as the strength of the material. We address here the main issue at the atomic scale: the understanding of the structure and mobility of isolated dislocations. We present a discrete model for the dynamics of dislocations in cubic metals. Numerical solutions of the model in 3D suggest that dislocations can be identified with discrete nonlinear waves. In simplified 1D and 2D geometries, we are able to obtain information about the depinning thresholds (dynamic and static Peierls stress) and the speed of the defects thanks to the analysis of traveling wave solutions of the discrete models.

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MS48
Elastic Crystals at Nonzero Temperature in Terms of Gibbs States

Elastic crystals are discussed in terms of Gibbs states of lattice models with non-compact "spins". An overview of known facts including an application of gradient Gibbs measures will be presented; remaining challenges will be mentioned.

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MS48
Crystallization in two dimensions

Why do solids frequently form crystals? In order to provide a mathematical answer a simple model consisting of N identical particles that interact with each other via a Lennard-Jones type pair potential is studied. Despite a strong degeneracy of the potential energy caused by the invariance under permutations it can be show that in two dimensions the ground state approximates a hexagonal lattice as N -¿ oo. The proof is based on carefully balanced geometric rigidity estimates combined with a quantificaton

of defect energies.

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MS48
Langevin Equations for Driven Lattice Systems

Exact Langevin equations for the height fluctuations in driven lattice growth models are derived from their master equations. The passage to the continuum limit is then considered for one- and two-dimensional substrates. The crossover at different length scales is compared with simulations for one-dimensional substrates. In two dimensions there are some quite intriguing results that suggest qualitatively growth as a function of the spatial dimension of the substrate.

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MS49
Mesoscopic Simulation for Surface Processes

Surface processes are multiscale phenomena which can be studied through mesoscopic models. Mesoscopic models are typically stochastic partial differential equations which are derived from the underlying microscale behavior. This talk begins with a brief description of these models. Then, new spectral computational schemes for stochastic partial differential equations will be introduced and validated using exactly solvable benchmark problems. Finally, some mesoscopic simulation results will be given.

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MS49
Dynamic Scaling and Chaos in Burgers Turbulence

Smoluchowski's coagulation equation describes some surprising coalescence processes. One of these is the solution to Burgers equation with random initial data. Coalescence here is the interaction between shocks. For example if one chooses a Brownian motion as initial data, the entropy solution for $t > 0$ has a dense set of shocks which can be described explicitly. Such self-similar initial data give rise to self-similar shock statistics. We would like to understand if these are typical. We build on work of Bertoin, to prove two rigorous results for a large class of random initial data. (a) Necessary and sufficient conditions for dynamic scaling. (b) A rigorous result on chaos. This is work with Bob Pego.

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MS49
Dynamic Scaling in Smoluchowski's Coagulation Equation

I'll describe a basic framework for studying dynamic scaling that links dynamical systems theory and probability theory. Smoluchowski's coagulation equation is a fundamental mean-field model for clustering. For the three simplest rate kernels, we can classify: all scaling solutions; all universality classes for scaling limits; all "infinitely divisible" size distributions; and we find scaling dynamics is chaotic in general.

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MS49
Self-similarity in Aggregation Problems with Continuous Input

We analyse Becker-Döring systems with continuous input of monomers and find the large-time asymptotic form of the cluster size-distribution function, which has an interesting self-similar structure. We also summarise the results for a system in which two morphologies of cluster grow, with one being subject to inhibition; the results of this analysis have important consequences for polymorph prediction.

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MS50
Phase Separartion in Diblock Copolymer Melts

Diblock copolymer melts, dubbed "designer materials", have the remarkable ability for self-assembly into various ordered structures. These structures are key to the many properties that make diblock copolymers of great

technological interest. In this talk, I will discuss modeling and analytical issues for both diblock copolymer melts and copolymer-homopolymer blends. Modeling issues pertain to deriving averaged density functional theories from the microscopic behavior of the polymer chains. Analytical work addresses these density functional theories with ansatz-independent results for energy minimizing configurations.

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MS50

Interfacial Patterns in Systems with Long-range Interactions of Coulomb type

This talk will present an overview of modeling, microstructure, and fluctuation phenomena in systems with competing short-range attractive interactions and long-range repulsive interactions of Coulomb type. Due to the fundamental character of Coulomb interaction, these systems arise in a wide range of applications, from polyelectrolytes and diblock copolymers to hight-T_c superconductors. We consider the situation in which the long-range interaction is a singular perturbation and introduce an interfacial reduction for the energetics on an infinite domain. This reduction allows one to study existence and stability of localized and periodic patterns in the appropriate singular limits, as well as the effect of thermal fluctuations.

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MS50

Double Gyroid Morphology of the Diblock Copolymer Problem

Micro-phase separation is driven by chemical incompatibilities between the different blocks that make up block copolymer molecules. In the diblock copolymer melt, the final equilibrium state then tends to be periodic mesostructures such as lamellar, column, spherical and double gyroid phases. It may be asked why do such morphologies occur in the mixtures? We would like to demonstrate the mechanism behind the appearance of the double gyroid (DG) phase on the basis of the gradient system with nonlocal effects and focus on the characterization of this intricate interconnected morphology of the Ia3d- symmetry.

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MS50

Nucleation in Fitzhugh-Nagumo System and Diblock Copolymer System

Nucleations play an important role in the coarsening and refining dynamics of microstructures in pattern forming systems. In this talk, we consider nucleations in two systems: the Fitzhugh-Nagumo system and the diblock copolymer system. Given any number of layers (say N) whose width is in the order ϵ, we construct solutions with K (¡N) spikes between the layers. We show that the Morse indeces of such solutions are at least K. Our construction uses Newton-type iterations in the Liapunov-Schmidt reduction. The spikes shift the layer locations in the order ϵ (for the FitzHugh-Nagumo system) or $\epsilon \log \frac{1}{\epsilon}$ (for the diblock copolymer system).

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MS51

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MS52

Direct Generation of Wannier-like Functions

(NMTO Minimal Basis Sets) from Multiple Scattering Theory and Applications

We describe how minimal basis sets may be generated directly. First, a set with the desired size and the desired characters of the individual functions is obtained by exact downfolding within multiple-scattering theory in real space. Secondly, this set of kinked partial waves, which exactly spans the solutions of Schrödinger's equation for an overlapping muffin-tin potential at a particular energy, is evaluated at a mesh of N+1 energies and superposed to form the desired minimal basis set. This set of N'th order Muffin Tin Orbials (NMTOs) is the polynomial approximation in the energy variable to the exact Hilbert space. Several current applications Wannier and Wannier-like functions generated in this way will be presented and possible future applications will be discussed.

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MS52

Predicting the Optical and Structural Properties of Matter at the Nanoscale

The properties of matter at the nanoscale are quite different than their macroscopic counterparts. For example, optical excitations in porous silicon are strongly blue shifted from crystalline silicon owing to quantum confinement. I will illustrate some recent theoretical progress in developing numerical approaches to compute the optical and electronic properties of semiconductor materials whose physical dimensions are on the nanoscale. I will focus on real space methods for solving the Kohn-Sham equation in this size regime.

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MS52

Bond-order Potentials: Bridging the Electronic to Atomistic Modelling Hierarchies

Robust interatomic potentials for simulating the growth of semiconductor films should be able to describe bond breaking and remaking naturally within their remit. In this talk we outline the derivation of such potentials by making two well-defined approximations within density functional theory (DFT). In the first step we demonstrate that a simple tight-binding (TB) bond model, in which the bond integrals are determined by the first principles TB-LMTO method, gives a good description of the DFT energetics of sp-valent systems such as Si or GaAs. In the second step we sketch the derivation of analytic bond-order potentials (BOPs) by coarse-graining the given TB electronic structure in terms of the moments of the local densities of states. The resultant sigma and pi bond orders have been shown to quantify the ubiquitous concept of single, double, triple and conjugate bonds in hydro-carbon systems and lead to a good treatment of radical formation. We discuss the current development of these potentials for modeling the MBE growth of GaAs films.

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MS52

Calculation of Free Energy Surfaces in Classical and ab initio Molecular Dynamics

The free energy surface of a complex system is usually characterized by the presence of deep minima separated by large barriers. Such minima correspond to distinct states of the system, and transitions among these minima reflect important changes such as phase transitions, chemical reactions and conformational modifications. Direct simulation of these processes is frustrated by the exponential dependence of the rate on the barrier height, and simulations often do not leave the free energy minimum from which they were started. In order to solve this problem we introduce a coarse-grained non-Markovian dynamics or metadynamics.

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MS53

Disclinations in Nematics Liquid Crystals

In the first part of the talk we analyse the static interactions between a nematic liquid crystal disclination and the surface of the half-space which bounds it. In particular, we show how the interaction depends on the surface extrapolation length: the nematic may expel the disclination if the anchoring strength is below a critical value. In the second part of the talk we describe the electrically-driven motion of a disclination.

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MS53

Nonlinear Elasticity of Liquid Crystal Gels and Applications to Cell Motility

Polysaccharides are electrolyte organic polymers capable of making gel phases upon hydration; in addition, their very unique shapes of elongated (helical, in some cases) chains allows such polymers to form liquid crystal phases. Con-

sequently, polysaccharide gels behave as anisotropic elastic solids. In the presence of water, the osmotic pressure in the gel causes swelling that results in very large volume expansions of the network. This phenomenon is due to electrostatic interactions between charged monomers in the network and free ions

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MS53

The Optomechanical Response of Nematic Elastomers

The salient feature of liquid crystal elastomers is the coupling between orientational order and mechanical strain. We present the results of experiments studying light-induced deformations in LC elastomers with dissolved dyes. Nematic LCEs doped with azo dyes show large (¿pi/6 bend) and fast (¡30ms) deformations; they also exhibit novel swimming phenomena. We discuss these results, and compare them with theoretical predictions, as well as with the results of numerical calculations.

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MS53

The Elasticity and Applications of Photoelastomers

Nematic elastomers strain, by 400% or more, when their order, Q, changes. Strain reverses when Q recovers. Order diminishes either by heating or, additionally in photo-elastomers, by illumination – photo-sensitive (dye) molecules can reversibly deform. Thus mechanical and optical responses map onto each other. Non-uniform illumination induces bending (for micro-actuation with beams), and mounds and troughs when writing optically. Bent beams have *two* neutral planes and a photo-curvature non-monotonic with penetration depth of the light.

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MS54

Remarks on the LSW theory of coarsening

We are working on an extension of the classical LSW theory of coarsening. As in previous work by others, we consider a "hierarchy" of theories of order $n = 1, 2, \ldots$, where n is the number of unknown distribution functions $f_1, f_2, \ldots, f_n$ in the theory. Each theory is based on a "closing assumption" which determines f_n as a functional of $f_1, \ldots, f_{n-1}$. The classical LSW theory is a theory of order $n = 1$. The ELSW theory that we are considering is a theory of order $n = 2$. I will be reporting on some very preliminary work with G. Fusco, G. Karali, and A. Terikas.

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MS54

Gelation in Coagulation and Fragmentation Models

We will give some results about the gelling of solutions to coagulation fragmentation models valid both in the discrete and continuous case. We will start with the coagulation equation and show in particular that all solutions gel in finite time if the homogeneity of the coagulationkernel is greater than one. We also give some estimates on the gelling profile. We then consider some coagulation-fragmentation equations and state some open problems.

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MS54

Continuum Description of Profile Scaling in Nanostructure Decay

We study the morphological relaxation of crystal surfaces below the roughening transition for diffusion-limited (DL) and attachment-detachment limited (ADL) kinetics. The slope profile is described by a PDE that accounts for line tension g_1 and step interaction energy g_3. We apply boundary-layer theory for self-similar shapes close to a facet. The boundary layer width varies as $(g_3/g_1)^{1/3}$ for DL kinetics and $(g_3/g_1)^{3/8}$ for ADL kinetics. These results agree with kinetic simulations.

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MS54

Coarsening in Topologically Complex Systems: Experiments and Simulations

We examine coarsening in two-phase mixtures that possess both positive and negative mean curvatures. We have employed three-dimensional phase field calculations in concert with three-dimensional reconstructions of the interfacial morphology to follow the evolution of a topologically complex dendritic microstructure during coarsening. The phase field method is used to determine the instantaneous interfacial velocities for a given experimental microstructure. A comparison between the results of the calculations and experiments will be given.

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MS55

Vector Riemann-Hilbert Problem Associated with Crack Propagation in a Viscoelastic Medium

A steady-state problem for a semi-infinite crack along an interface between rigid and viscoelastic half-planes is analyzed. The problem is equivalent to a vector Riemann-Hilbert problem with a 2×2 matrix coefficient which has branch points. A method for it solution is proposed. It reduces the vector problem to a scalar Riemann-Hilbert problem on a 4-sheeted Riemann surface whose solution is found in terms of a solution of a singular integral equation with the Hensel-Landsberg kernel.

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MS55

Intersonic Crack Propagation along a Weak Plane in Solids

The fundamental solution for a pair of concentrated shear loads acting on the crack faces, while the crack tip starts to propagate intersonically, is obtained. The transient solution is also found for an intersonically moving crack tip that is suddenly arrested after propagating some distance. Unlike subsonic crack growth, the stress intensity factor does not reach the static value instantaneously once the intersonically propagating crack tip is arrested. Instead, it only approaches the static value asymptotically.

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MS55

Laboratory Earthquakes

We report on the experimental discovery of the phenomenon of, spontaneously nucleated, supershear rupture and on the visualization of the mechanism of subRayleigh to supershear rupture transition in frictionally held interfaces. Highly instrumented experiments mimicking crustal fault rupture events are used to study model earthquakes in a controlled laboratory environment. The experiments, motivated by recent seismological reports of supershear fault rupture, probe the parameter space governing the physics of dynamic rupture of incoherent interfaces.

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MS55

Corrugation Waves?

A "crack front wave" is a perturbation of the leading edge of a propagating crack, in the plane of propagation, which propagates without attenuation along the crack edge. It was discovered computationally and its existence was confirmed (with some explicit restrictions) from analytic formulae for the perturbation. A "corrugation wave" corresponds to an out-of-plane perturbation. The requisite analytic formulae are available, and will confirm (or not) whether such a wave exists. The evidence so far is that it does not, but when the crack speed is large enough the perturbation decays only slowly as it runs along the crack edge.

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MS56

The Effects of Applied Current on Growth Forms of Crystals

Numerical solutions to a phase field model of single crystal growth with electric current are presented. Results show current affects interface stability and can accelerate or decelerate the solidification rates of features such as dendrite tips. Regularization of secondary branching occurs by current pulsing and depends on the orientation of applied current. Extension of the work to the treatment of dilute binary alloys and to the development of more suitable far-field boundary conditions will be discussed.

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MS56

Models for Additive Effects on Microstructure and Surface Morphology During Electrodeposition

Common experience shows that the microstructure and surface roughness of electrodeposited (ED) films can be controlled by adding small quantities of molecular "additive" species to the electrochemical bath. In the first part of the talk I will describe how linear stability analysis provides a natural framework to understand and quantify how a class of additives ("levellers") reduce surface roughness of the growing film. In the second part of the talk I will discuss our efforts to understand the effects of another class of additives ("grain refiners") on the time-dependent microstructure of the growing film. We address this issue by carrying out kinetic Monte Carlo simulations of a modified Potts model.

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MS56

Phase-Field Model of Electrochemistry

We describe a phase-field model for a simple electrochemical system consisting of an electrode and electrolyte separated by a diffuse electrochemical interface. The thermodynamic treatment is based on a four-component ideal solution model, augmented by a phase-field variable that varies through the interfacial region. Under equilibrium conditions,the model predicts the charge separation associated with the double layer at the interface, the associated electrocapillary curve (surface energy versus potential), and the decay length of charge in the electrolyte as a function of electrolyte concentration. The model also provides a description of kinetic behavior during planar deposition or dissolution of the interface by an applied current.

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MS56

Formation of Regular Nano-Porous Structures During Anodization of Aluminum

Spontaneous formation of spatially-regular hexagonal arrays of pores in a growing layer of alminum oxide during anodization of aluminum is studied. It is shown that the growing layer of aluminum oxide can become unstable due to strong (exponential) dependence of the current on the overpotential (Butler-Volmer relations) and the coupling between the two interfaces: metal-oxide and oxide-electrolyte. This instability is long-scale and leads to the growth of pores. We show that hexagonal spatial ordering of pores can be a result of elastic stresses produced in the aluminum oxide layer during its growth. Numerical simulations of a model nonlinear evolution equation confirm this conclusion.

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MS57

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MS57

Simple Stochastic Models of Motor Protein Dynamics

Motor proteins, or molecular motors, are enzymes that transform a chemical energy into mechanical motion. They play important role in functioning of biological cells. Current experimental techniques allow to measure the biochemical and mechanical properties of single motor protein molecules with great precision. We develop a set of simple discrete-state stochastic models, which provide exact and explicit expressions for properties of motor proteins. This approach allows us to describe fully the existing experimental data on dynamics of different molecular motors. The advantages of this theoretical method are its simplicity, the ability to obtain exact solutions, and the possibility to account for complex biochemical mechanisms. Thus it may provide a quantitative basis for investigation and under-

standing distinct motor proteins.

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MS58
From Atoms and Defects to Kinetic Relations

The kinetics or laws govering the dynamics of phase boundaries has been a topic of active research in a variety of settings. It has an important role in the hysteretic behavior of materials. It is also related to non-classical shocks in hyperbolic convervation laws and the entropy conditions that one needs to study them. This talk is related to the kinetics of twin boundaries in materials that undergo martensitic phase transformation and describes the progress in a program of research that tries to obtain the kinetic laws starting from relevant microscopic physics.

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MS58
Dynamic Transitions in Bistable Lattices

Discrete one- and two-dimensional lattices consisting of point particles connected by bistable bonds are considered. The bonds follow a trimeric piecewise linear force–elongation diagram of a general view. Initially, Hooke's law is valid as the first branch of the diagram; then, when the elongation reaches the critical value, the other comes in force. The latter branch can be parallel with the former (mathematically this case is simpler) or have a different inclination. Steady-state transition waves are examined. For a prestressed two-dimensional lattice the dynamic transition is found as a wave localized between two neighboring lines of the lattice particles. The transition wave itself and dissipation waves carrying energy away from the transition front are described. The transition wave speed as a function of the prestress is found. It is also found that, for the case of the transition leading to an increased tangent modulus of the bond, there exists non-divergent tail waves exponentially localized in a vicinity of the transition line behind the transition front. The previously obtained solutions for crack dynamics in lattices appear now as a partial case corresponding to the second branch having zero resistance. At the same time, the lattice-with-a-moving-crack fundamental solutions are essentially used here in obtaining those for the localized transition waves in the bistable-bond lattices. For the piecewise linear diagram, where the transition point is that of a jump discontinuity, explicit analytical solutions are found, while for a general path of the transition, the problem is reduced to an integral equation. The results are compared to the ones obtained for a continuous elastic model and for a related version of one-dimensional Frenkel-Kontorova model. The discrete models allow the following to be obtained: (a) a closed formulation for the transition process, (b) the transition wave speed as a function of external actions, (c) the total speed-dependent dissipation and the dissipation wave structure, and (d) the non-divergent exponentially localized waves.

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MS58
Lattice Model of Plastic Deformation

We present a simple mechanical model whose microscopic dynamics is of a gradient flow type while homogenized macroscopic response is similar to rate-independent plasticity. The basis of the model is a lattice of interacting elastic elements with non-convex energies.

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MS58
Explicit Kinetic Relation from "First Principles"

We study a fully inertial lattice model of a martensitic phase transition which takes into account interactions of first and second nearest neighbors. Although the model is Hamiltonian at the microscale, it generates a nontrivial macroscopic relation between the velocity of the martensitic phase boundary and the driving force of transformation. The apparent dissipation is due to the induced radiation of lattice waves carrying energy away from the front.

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MS59
Smectic Phases with Cubic Symmetry: Layered Systems with High Intrinsic Curvature

Smectic blue phases have quasi-long range smectic translational order as well as three dimensional crystalline order. We propose a construction which fills space by adding

layers on top of a minimal surface, introducing either curvature or edge defects as necessary. We find that for the right range of material parameters, the favorable saddle-splay energy of these structures can stabilize them against uniform layering. The optimal construction balances frustration between layer compression, mean curvature and saddle-splay. As with traditional blue phases, the curvature frustration results in a lattice of topological defects, which is why these phases only appear near the isotropic transition.

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MS59

Numerical Modeling of Frustrated Nematic Twist Cells

Within the Landau-de Gennes theory of liquid crystals, we study the equilibrium configurations of a nematic cell with twist boundary conditions. At a sufficiently narrow cell gap (on the order of the biaxial coherence length), "twist-like" solutions will cease to be found for the symmetric case of 90-degree total twist. The free-energy minimizing configuration will instead undergo a local biaxial transformation or "eigenvalue exchange," as has been realized in several other settings with highly strained nematics. For the case of perturbed boundary conditions (different from 90 degrees), the symmetry of the problem is broken, and it is less clear what to expect. We use numerical bifurcation analysis to obtain a complete picture for this case.

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MS59

On the Defect Dynamics in Nematic Liquid Crystals

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MS59

Homogenization Estimates for Polydomain Nematic Elastomers undergoing to Large Deformation

We make use of "linear comparison" homogenization techniques to estimate both the effective mechanical response and the evolution of the domain textures in polydomain LCEs. For this purpose, we use the self-consistent approximation for the relevant linear comparison composite, which allows the incorporation of two-point statistical information leading to information also on the field fluctuations within the sample. Finally, we study the stability of the deformations, by checking the strong-ellipticity condition of the relevant incremental moduli.

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MS60

A Kinetic Model for a Step Edge

Epitaxy is the growth of a thin film by attachment to an existing substrate in which the crystalline properties of the film are determined by those of the substrate. Epitaxial thin films grow by attachment of adatoms to step edges (or island boundaries). In contrast to the assumptions of classical models, the state of a step edge is typically in a kinetic steady state that is far from equilibrium. This talk presents a detailed model for the dynamics of a step edge, along with analysis of the model in several limits, and a discussion of equilibrium for this system. The model is partially validated by comparison to results from kinetic Monte Carlo simulations. For large adatom diffusion, the asymptotics of this model includes edge diffusion and line tension, providing an atomistic, kinetic derivation of the Gibbs-Thomson formula.

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MS60

A Fourth Order Accurate Discretization for the Laplace and Heat Equations on Arbitrary Domains, with Applications to the Stefan Problem

In this talk, we will first describe a fourth order accurate finite difference discretization for both the Laplace equation and the heat equation with Dirichlet boundary conditions on irregular domains. In the case of the heat equation we use an implicit discretization in time to avoid the stringent time step restrictions associated with requirements for explicit schemes. We then turn our focus to the Stefan problem and construct a third order accurate method that also includes an implicit time discretization. Multidimensional computational results are presented to demonstrate

the order accuracy of these numerical methods.

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MS60

Grain Boundary Diffusion Due to Stress and Electromigration

The stress driven grain boundary diffusion problem is a continuum model of mass transport phenomena in microelectronic circuits due to high current densities (electromigration) and gradients in normal stress along grain boundaries. The model involves coupling many different equations and phenomena, and difficulties such as non-locality, stiffness, complex geometry, and singularities in the stress tensor near corners and junctions make the problem difficult to analyze rigorously and simulate numerically. We present a new approach to this problem using techniques from semigroup theory to represent the solution, and study the problem numerically using a singularity capturing least squares finite element method.

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MS60

Level Set Simulations of Dislocation-particle Bypass Mechanisms

Dislocations are line defects in crystals. Their motion carries the plastic deformation. Particle dispersions strengthen metals by acting as barriers to the motion of dislocations. We present the results of full three-dimensional dislocation dynamics simulations for dislocation bypassing particles. The simulation method is based on the level set method, that naturally accounts for the topological changes and three dimensional motion of dislocations. The simulations show a wide range of bypass mechanisms, including particle cutting, dislocation loop formation and combinations of these. Some of the bypass mechanisms are classical and others have never been reported previously.

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MS61

High order asymptotics and perturbation problems for 3D interfacial cracks

We present an asymptotic algorithm for analysis of a singularly perturbed problem in a domain containing an interfacial crack. The crack is assumed to be flat, and its front, initially straight, is perturbed in the plane containing the crack. The algorithm requires two-term asymptotics of the matrix weight function and two-term asymptotics of the physical field. It is aimed to determine an explicit asymptotic representation of the stress-intensity factors near the edge of a "wavy" crack.

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MS61

Wave of Transition in Chains and Lattices from Bistable Elements

The paper investigates dynamics of structures from bistable elements that are able to dissipate energy of an impact by distributing a "partial damage" over a large area and by quickly transforming the energy into high-frequency dissipative modes. We analytically describe damage waves and multiple equilibria in partially damaged chains and lattices, conditions of propagation and controllability of the damage, and an adequate "dynamic homogenization."

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MS61

A Solution Method for Dynamically Accelerating Cracks in Viscoelastic Materials and Elastic Bimaterials

We will discuss a general solution method for a dynamically accelerating crack in a linear viscoelastic material or along an interface in an elastic bimaterial. This solution method is based on a transform method developed by L.I. Slepyan for solution of dynamic elastic fracture problems. The analysis includes an exact, closed-form expression for the stress intensity factor for an arbitrary time dependent crack face traction. This work has been done in collaboration with Jay R. Walton.

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MS61

Dynamic Steady-state Crack Propagation in Anisotropic Viscoelastic Material

Presented here is a framework utilizing Fourier transform and complex variable methods for carrying out a rigorous analysis of a semi-infinite generalized plane strain crack propagating in a general anisotropic linear viscoelastic body. In general, the method requires the solution of a matrix Riemann-Hilbert problem. For an instropic body or a transversely isotropic body, the matrix problem uncouples resulting in three scalar Riemann-Hilbert problems which can be solved analytically even when Poisson's ratio is not assumed constant.

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MS62

Electrokinetic Phenomena Due to AC Faradaic Charging

We report our study of nonlinear and non-equilibrium electrokinetics driven by Faradaic electrode polarization, which can produce a surface AC electro-osmotic velocity several orders of magnitude higher than the Smoluchowski slip velocity. We examine the dynamic ion and field distributions within the polarized region by matched asymptotics and time averaging. An effective boundary condition involving time derivatives is then obtained for the external complex Laplace equation. For a planar geometry and linearized boundary conditions, analytical solutions are obtained by Fourier transform and conformal map.

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MS62

Fluid Flow and Dispersion in the Electrophoretic Separation of Biomolecules

Capillary Electrophoresis (CE) is an efficient method for separating mixtures of chemical species by exploiting differences in their electrophoretic mobility in an applied electric field. It is an important tool of biochemical analysis in the health sciences, biological sciences and forensics. The problem of determining axial dispersion of the sample will be discussed. This determines the resolution and sensitivity of a CE system. Thus, minimizing the axial dispersion is often the primary design objective.

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MS62

Ion Exchange Funneling

Inexpensive heterogeneous ion exchange membranes are prohibitively polarizable for use in electrodialysis. According to recent experiments, polarizability of these membranes may be considerably reduced by casting on their surface a thin layer of crosslinked polyelectrolyte, weakly charged with the same sign as the membrane's charge. It is shown, based on the proposed model of modified membrane,that the effect of membrane modification follows from 'funneling' of counterions by the charged layer towards the permeable sites of the membrane.

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MS62

Electroconvection in Concentration Polarization

Electro-convection is reviewed as a mechanism of mixing in the diffusion layer of a strong electrolyte adjacent to a charge-selective solid, such as ion exchange membrane. Two types of electro-convection in strong electrolytes may be distinguished: bulk electro-convection or convection induced by electro-osmotic slip of either quasi-equilibrium or non-equilibrium type. According to recent studies, the latter appears to be the likely source of mixing in the diffusion layer, leading to 'over-limiting' conductance in electrodialysis.

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MS63

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MS63

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MS63

Analytic models for mechanotransduction: gating a mechanosensitive channel

Analytic estimates for the forces and free energy generated

by bilayer deformation reveal a compelling and intuitive model for MscL channel gating analogous to the nucleation of a second phase. We argue that the competition between hydrophobic mismatch and tension results in a surprisingly rich story which can provide both a quantitative comparison to measurements of opening tension for MscL when reconstituted in bilayers of different thickness and qualitative insights into the function of the MscL channel and other transmembrane proteins.

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MS64

A Global Bifurcation Approach to Two-Phase Equlibria in Elastic Solids

We consider multi-phase equilibria of elastic solids under loading. A well known approach to this class of problems is to infer micro-structure via minimizing sequences of the potential energy. In spite of its successes, that method allows "infinite refinement" of phase mixtures, it ignores equilibrium conditions and it is not easily generalized to problems with loading. Instead, we propose the use of global bifurcation, in the presence of small inter-facial energy, to determine paths of equilibria. We present results for a model "two-well solid" of rectangular cross-section in anti-plane shear. We establish the rigorous existence of global bifurcating branches of equilibria, with each branch having the precise symmetry of a certain eigenfunction of the linearization. We then perform global-numerical path following in appropriate fixed-point spaces (according to the known symmetry of a given branch), i.e., the orientation of our mesh is prescribed by the symmetry. We treat both (the reciprocal of) the capillarity coefficient and the magnitude of the boundary displacement as continuation parameters. In this way we obtain branches of phases, and phase-tip splitting at the boundary.

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MS64

Travelling Waves in a Discrete Chain with Bi-stable Springs: A Model for Martensitic Solids

Martensitic materials exist in multiple metastable phases under the same conditions of temperature and stress. The interfaces between these phases are mobile and their motion endows these materials with interesting mechanical properties such as shape-memory. A continuum description of these materials is inadequate to understand the mobility of the interfaces. Usually one postulates a kinetic law relating the thermodynamic driving force across the interface to its velocity. We motivate this kinetic law from a microscopic model based on atomic scale physics. We study travelling waves in a one dimensional chain with bistable potentials and show that data from a variety of simulations collapses onto a single curve representing a kinetic law in the continuum sense.

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MS64

Dispersion, Dissipation and the Kinetic Relation for a Dislocation

We study the uniform motion of a screw dislocation. The Peierls-Nabarro formulation has been adopted to model the dislocation. We present certain higher gradient and dynamic higher gradient continuum models involving length scales that modify the dispersion relation of the classical continuum model for elastic materials. We construct the displacement field for such elastic models and obtain the kinetic relation. In these conservative models the dissipation at macroscale occurs due to the generation of waves at microscale.

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MS64

A Probabilistic Approach to Transient Pattern Formation

Many complicated patterns are generated by transient processes depending on a small parameter, and one is generally interested in establishing lower bounds on the pattern amplitudes as this parameter approaches zero. Recent results on spinodal decomposition in Cahn-Hilliard models have produced such bounds. Unfortunately, they exhibit a dimension dependence which seems unavoidable from a theoretical viewpoint, but cannot be observed in practice. In this talk I present a probabilistic approach which resolves this apparent paradox.

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MS65

Disclinations in a Homogeneously Deformed Nematic Elastomer

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MS65

Landau-de Gennes Model of Liquid Crystals and Critical Wave Number

Landau-de Gennes model has been used to describe phase transitions from nematic to smectic liquid crystals. Minimizers of some variational problems of the model exhibit interesting concentration behaviors and critical phenomena, some of which will be discussed in this talk.

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MS65

Analytic Aspects of Phase Transitions in Liquid Crystals

We investigate a model used to describe equilibrium configurations near the nematic-smectic phase transition. As the temperature is lowered through this threshold configurations with nematic structure loose their stability and configurations with a layered (smectic A) structure are energetically preferred. We study minimizers to the Chen-Lubensky model, which couples the Frank energy for the director with a Ginzburg Landau energy for a complex-valued order parameter. The parameter accounts for the additional layering in the smectic phase. This is a nonlinear first order elliptic energy. We investigate the nature of solutions and the manners in which the Frank and chirality constants in the energy affect the transition temperature and trigger a phase transition. We also relate this investigation to recent work on phase transitions between nematic and smectic C phases by S. Joo, which are described by second order energies.

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MS65

Effect of Random Field Disorder on N-I Transition

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MS66

A Two-Dimensional Finite Element Method for Simulating Microstructure and Constitutive Response of Polycrystals During HIgh Temperature Plastic Deformation

We describe a finite element method designed to model the mechanisms that cause superplastic deformation. Our computations idealize the solid as a collection of two-dimensional grains, separated by sharp grain boundaries. The grains may deform plastically by thermally activated dislocation motion, which is modeled using a conventional crystal plasticity law. The solid may also deform by sliding on the grain boundaries, or by stress driven diffusion of atoms along grain boundaries. Our computations can also account for diffusion along surfaces in the solid, and can therefore be used to simulate the behavior of thin strips or films, or to model diffusive or plastic void growth in the solid. Finally, all the grain boundaries may migrate, driven by grain boundary energy, or stored elastic energy in the grains themselves. The governing equations are solved using a finite element method, which includes a front-tracking procedure to track the evolution of the grain boundaries and surfaces in the solid. The method is used to solve several representative boundary value problems. To demonstrate the convergence and accuracy of the method, we model the growth of a periodic array of cavities on a grain boundary, and compare the predictions of our computations with the analytical solution to this problem. To illustrate the capabilities of the method, we model the behavior of a small assembly of grains under conditions intended to represent superplastic flow. We compute the evolution of the solids microstructure; representative stress-strain curves; and the strain-rate sensitivity of the solid as a function of temperature and strainrate. In addition, we compute the relative contributions to the plastic strain from grain boundary sliding, diffusion and slip in the grains as a function of strain rate and temperature. The results show encouraging qualitative and quantitative agreement with experimental observations.

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MS66

An Efficient Method for Tracking Interfaces in 3D Homogeneous Media

The evolution of microstructures produced by diffusional transformations in elastically stressed binary alloys is simulated using boundary integral method. The elastic stress is induced by the misfit between the lattice parameters of the two phases. We discuss an efficient method to compute

the elastic energy, which overcomes the difficulty caused by the lack of the explicit formula for 3D anisotropic Green's function. We also compare the method to alternative methods for solving the elasticity problem.

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MS66

Adaptive simulation of Microstructured Materials: Multiphase Flows

Microstructured materials, such as emulsions and polymer blends, crystals and metallic alloys, blood and biological tissues, are fundamental to many industrial and biomedical applications. These diverse materials share the common feature that the microscale and macroscale are linked. The phenomena at the micro scale, such as the morphological stability of crystalline precipitates and drop deformation, break-up and coalescence determine the microstructure and its time evolution; thus affecting the rheology and mechanical properties of the materials on the macro scale. In this talk, I will focus on a modeling effort to describe fluid flows with deformable interfaces on the micro scale. The models are physically based and are capable of describing a wide variety of interface phenomena including interface pinchoff and reconnections. We will validate the models by comparisons to theory and experimental results for a number of different fluid flows. We discuss practical issues associated to the model as well as the incorporation and effectiveness of adaptive mesh refinement.

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MS66

Numerical Methods for Material Transport with Global Dynamics

An Eulerian framework for treating material tranposrt on a moving interface is presented. Moreover the material concentration on the interface changes the interfacial property and influences the global dynamics. Our method is able to couple these effects together with the global dynamics.

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PP1

Closure of the Set of Diffusion Functionals and That of Elasticity

We determine the closure for Mosco-convergence in $L^2(\Omega, \mathbb{R}^3)$ (resp. $L^2(\Omega)$) of the set of elasticity functionals (resp. *set of diffusion functionals*). We prove that this closure coincides with the set of all non-negative lower-semicontinuous quadratic functionals which are objective, i.e. which vanish for rigid motions (resp. *set of all Dirichlet forms*). The result is still valid if we consider only the set of isotropic elasticity functionals which have a prescribed Poisson coefficient.

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PP1

A Discrete Model for the Elastic Field of a Surface Step

The method of lattice statics is applied to an epitaxial system with fully atomistic potentials. Lattice mismatch and intrinsic surface stress are naturally built in as sources of stress, as is standard in models of heteroepitaxy. By choosing the strain relative to an appropriately chosen reference lattice, analytical formulas for the effective force field or traction of a step are derived, and for the macroscopic monopole and dipole forces due to the step. The results provide an atomistic validation of the Marchenko-Parshin for the dipole moment in terms of the elastic surface stress.

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PP1

A System of A Pde Coupled with A Variational Inequality

One approach in Hele-Shaw problems for manufacturing processes in composites is the variational inequality method. We present the existence of solutions to a new kind of nonlinear systems. In this system a nonlinear variational inequality is coupled with a nonlinear partial differential equation. To the best of our knowledge, nonlinear systems of a partial differential equation coupled with a variational inequality have not been studied. One of our principle difficulties is to obtain a priori estimate of the critical growth. We circumvent this difficulty by invoking

the reverse Hölder inequality.

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PP1

Disorder Effects in Photonic Crystal Structures

This work examines the effects of disorder in photolithographically manufactured photonic bandgap structures. The effects of variation in feature size and shape are examined computationally using disorder information extracted from real micrographs. A real-space analysis of Maxwell's equations in 2-D is carried out using the finite element method, with performance quantified in terms of energy flux through a structure. Results show the geometric features that are most critical to performance of photonic waveguide devices.

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PP1

Algorithms for Classical Density Functional Theory

We have developed algorithms for solving 2D and 3D nonlocal classical density functional theory. Classical DFT predicts equilibrium behavior for confined molecular fluids, including complex phase transition and self-assembly. The computational problem is the minimzation of an energy functional, which contains nested moderate-range integrals. To efficiently solve the model for 2D and 3D geometries, we have implemented a parallel solution strategy that includes domain decomposition, heuristic load balancing, a Newton method with analytic Jacobian, and a preconditioned Krylov iterative solver. The solution space is analyzed using parameter continuation algorithms. The algorithms have enabled the rapid anaysis of manyinteresting nanoscale systems, including capillary condensation in porous media and block co-polymer self-assembly.

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PP1

Comparison of Models for Frontal Polymerization

We analyze numerically and analytically both exact and approximate systems of PDEs/ODEs that correspond to a single-step model of frontal polymerization. We show that, unlike for similar gasless combustion models, the models that employ piecewise-defined approximations of Arrhenius kinetics can lead to inaccurate long-time behavior of solutions. Further, we show that for rapidly advancing polymerization fronts, residual amounts of monomer left behind the front subsequently disappear through the bulk polymerization.

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PP1

A Biphasic Model for Local Cell-Matrix Mechanics in Articular Cartilage

Deformation in the local cell-matrix unit of articular cartilage is considered. The cell and its pericellular matrix (PCM) are idealized as linear isotropic biphasic continua with spherical geometry. Solutions of the associated interface problem are employed in a parametric analysis of transmission of transient-free radial displacement, solid stress and strain. The dual role of the PCM as a transmissive and protective layer is assessed with varying pericellular stiffness and permeability in normal and osteoarthritic models.

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PP1

Effect of Surface-Energy and Wetting Interaction Anisotropy on Self-Organization of Quantum Dots

We consider the spontaneous formation of quantum dots in a thin solid film caused by anisotropic surface-energy and wetting interactions with the substrate. We show that wetting interactions change the spectrum of the faceting instability and can lead to the formation of spatially regular patterns of quantum dots. We derive amplitude equations that describe the weakly nonlinear evolution of the patterns and study the effects of anisotropy on the pattern stability.

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PP1

Atomistic and Continuum Models of Crystalline Solids

We present the following results: 1. Existence of local minimizers for the continuum models obtained from the Cauchy-Born rule; 2. The full atomistic model has a solution nearby, and we give estimates for the difference. The above results are obtained for a variety of atomistic models, and we believe they give a satisfactory description on the relation between atomistic and continuum models for defect-free solids at zero temperature. As applications, we discuss: 3. Error estimates for the local quasi-continuum method; We will also discuss the problem with defects.

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PP1

An Efficient Algorithm for Fracture Simulations

This paper presents an efficient algorithm for the simulation of progressive fracture in disordered quasi-brittle materials using discrete lattice networks. The main computational bottleneck involved in modeling the fracture simulations using large discrete lattice networks stems from the requirement to solve *a new large set of linear equations* every time a new lattice bond is broken. To address this problem, we propose an algorithm that is based on multiple-rank sparse Cholesky downdating algorithm. Using the present algorithm, the computational complexity of solving the new set of linear equations after breaking a bond reduces to a simple *backsolve* (forward elimination and backward substitution) *using the already LU factored matrix.* That is, the computational cost is $O(nnz(\mathbf{L}))$, where $nnz(\mathbf{L})$ denotes the number of non-zeros of the Cholesky factorization $\mathbf{L}$ of the stiffness matrix $\mathbf{A}$. This algorithm using the direct sparse solver is faster than the Fourier accelerated iterative solvers such as the preconditioned conjugate gradient (PCG) solver, and eliminates the *critical slowing down* associated with the iterative solvers that is especially severe close to the percolation critical point.
Numerical results using random resistor networks for modeling the fracture and damage evolution in disordered materials substantiate the efficiency of the present algorithm. Using this algorithm, for the first time, we simulate the fracture of a two-dimensional 1000×1000 triangular lattice system. Based on these numerical simulations that span two orders of length scales, we propose scaling laws for damage evolution in disordered brittle materials.

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PP1

Dynamics of the Morphological Evolution of Sputter Ripples

The evolution of sputter ripples provides a means of testing theoretical models of surface evolution. We use a variational model to study the non-linear and singular nature of the equations that govern the evolution of crystalline surfaces below the roughening temperature and apply the method to realistic systems in different kinetic regimes. The inherent non-linearity of the problem does not allow for simplistic predictions of exponential or non-classical inverse-linear decay of the ripple amplitude. Other possible metrics could be the integrated power spectral density or the peak intensity.

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PP1

Development of a Micro-Macro Simulation Algorithm for Polymeric Fluids

A micro-macro algorithm for the simulation of polymeric flow is developed. The algorithm couples the mass and the momentum balance equations from continuum mechanics with a microscopic-based rheological model in which polymer stress depends on the molecular dynamics as represented by two stochastic processes. The balance equations are solved using finite element techniques, while the polymer stress is computed using stochastic simulations. Numerical results in the contraction domain are presented and comparisons are made with experiments.

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PP2

Identification of NiTi Alloy Thermal Expansion Coefficient Using Preisach Density Function.

In this paper we develop a empirical relation between the density function of the Preisach Operator and the thermal coefficient of expansion of a NiTi alloy. A thermodynamical basis for the relation is established and experimental data is used to verify the relation.

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PP2

Kinetics of Average $\mathcal{N}$-Hedra in 3-D Networks

An analysis is developed for 3-d space-filling networks (foams and polycrystals) that satisfies space filling, equilibria at triple lines and quadrajunctions, volume conservation, and motion by mean curvature. The rates of volume change for polyhedra in 3-d networks depend linearly on the integral Gaussian curvature and mean curvature—quantities that can be determined *exactly* for average $\mathcal{N}$-hedra. Comparisons with evolution kinetics found for irregular networks simulated with Surface Evolver are in agreement with theoretical predictions.

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PP2

Estimating the Mechanical Properties of Amorphous Columnar Thin Films Using Md

We present a Lagrangian-based MD approach for determining the constitutive equations of a columnar amorphous thin film. The Lagrangian formalism differs from Parrinello-Rahman-type as it is based on homogenization concepts valid for a continuous media in a regime of large deformation and far from quasi-static equilibrium conditions. Our interest lies in describing the effective properies of a porous thin films with a columnar microstructure that have been produced via MD simulations.

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PP2

Mathematical Analysis of a Simple 1D Discrete-Continuum Method for Materials Simulation.

The description and computation of fine scale localized phenomena arising in a material (in nanoindentation experiments, for instance) is a challenging problem that has given birth to some multiscale methods. In this talk, we propose a mathematical analysis of a simple 1D method which couples two scales, the atomistic one and the continuum mechanics one, into a single model.

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PP2

Mesh Optimization for the Quasicontinuum Method: A Generalization of Vale to Inelastic Problems

The current formulation of the Quasicontinuum (QC) method, with its seamless bridging of length scales, relies on a static triangulation of the reference crystal configuration. The computational mesh needs to encompass a wide range of spatial resolutions, from fully atomistic at defect cores, to continuum-like in defect-free regions. Moreover, it must continously adapt to the structure of the deformation field, so as to return the least possible potential energy for a fixed number of nodes. To this end, the mesh adaption process has been usually governed by some form of empirical indicators. In this work, we present an extension of the Variational Adaptive Lagrangian-Eulerian (VALE) method into the QC context. In the spirit of VALE, the computational mesh is factored directly into the description of the energetics of the crystal. Therefore, the potential energy minimizer determines not only the equilibrium configuration of the crystal, but also the optimal configuration of the computational mesh. We apply the VALE-QC method to the investigation of early stages of plastic deformation during nano-indentation, void growth or dislocation emission at a crack tip in single crystals.

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PP2

Mathematical Models of Aerogels

Aerogels are modeled by intersecting excursion sets of independent Gaussian random fields. These fields are obtained by matching small-angle neutron scattering (SANS) data with the scattering function for the model. The chord-length functions, which contain partial clustering information, are then computed for the model. Visualizations of this model are compared to electron microscopy images and gas adsorption pore size distributions. A long-term goal is to discriminate between open and closed porosities.

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PP2

Fatigue Behaviour of Ferroelectrics

Up to now, the large actuation strain displayed by ferroelectrics could not be fully exploited mainly due to fatigue

phenomena at low cycles number. To understand better these phenomena, and possibly improve behaviour of ferroelectrics, we propose a finite elements simulation scheme to enable the computation of the response under cyclic loading. The coupled system of PDEs includes a time-dependent Guinzburg-Landau approach for the polarization problem and a cohesive zone model for the mechanical problem.

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PP2

Equilibrium Shapes of Epitaxially Strained Islands with Finite Contact Angle

The equilibrium shape of an epitaxially strained thin film island located on an elastic substrate is determined. The island is assumed to have a nonzero contact angle at the film/substrate/vapor contact line. The equilibrium shapes depend on the surface energy of the film interface and the lattice misfit strain at the film-substrate interface. This elastic problem is solved in the limit of the small slope approximation. Assuming that the elastic constants in the film and substrate are equal, the problem for the interface shape can be reformulated as an integro-differential equation. This equation is discretized and solved numerically for different values of the misfit, contact angle and surface energy. Equilibrium shapes of two and three dimensional islands are computed. Multiple hump and non-axisymmetric solutions are found for various values of the parameters.

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PP2

Full Two-Scale Expansion for Nonlinear Periodic Problems and Higher-Order Homogenized Problems

For a scalar uniformly elliptic nonlinear periodic homogenization problem, with "outer" periodicity conditions and natural growth of the energy function, we construct a full asymptotic expansion, which has a precise "double-series" structure, separating the slow and the fast variables "in all orders". The error bounds are proved. The first "essentially nonlinear" term in the higher-order homogenised equations has the form of a fully nonlinear operator which in the dimension two is of Monge-Ampère type. The slowly varying part of the full asymptotic expansion is the asymptotics "in all orders" for the actual solution. Applying then variational truncation we construct "higher-order" homogenised equations. We prove that at least under some further natural "non-degeneracy" assumptions it has a solution (the existence), and that any such solution is close to the actual solution in appropriate norms. Higher-order effects are related to those nonlocal when the uniform ellipticity condition is relaxed.

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PP2

Effective Thermal Expansion of Multiphase Heterogeneous Medium.

The problem of the effective expansion of a heterogeneous medium due to a temperature change or phase transformation is considered. For this purpose a differential scheme is developed for estimation of effective thermoelastic properties of multiphase statistically homogeneous composites. The effective thermal expansion coefficients are found to be sensitive to the composite microgeometry. Variational methods are applied to estimate the bounds for the effective thermal expansion. The work is carried in collaboration with Prof. Z.Hashin, Tel Aviv University, Israel.

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PP2

Finite Element Simulations for the Burton-Cabrera-Frank Equations

An adaptive finite element method is developed for a class of free boundary problems modeling island dynamics in epitaxial growth. Such problems consist of an adatom (adsorbed atom) diffusion equation on terraces of different height; boundary conditions on terrace boundaries including the kinetic asymmetry in the adatom attachment and detachment; and the normal velocity law for the motion of such boundaries determined by a two-sided flux, together with the one-dimensional edge diffusion. The problem is solved using two independent meshes: a two-dimensional mesh for the adatom diffusion and a one-dimensional mesh

for the boundary evolution. The diffusion equation is discretized by the first-order implicit scheme in time and the linear finite element method in space. A technique of extension is used to avoid the complexity in the spatial discretization near boundaries. All the elements are marked, and the marking is updated in each time step, to trace the terrace height. The evolution of the terrace boundaries includes both the anisotropic mean curvature flow and the anisotropic surface diffusion. Its governing equation is solved by a semi-implicit front-tracking method using parametric finite elements. Simple adaptive techniques are employed in solving the adatom diffusion as well as the boundary motion problem. Numerical tests on pure geometrical motion, mass balance, and the stability of a growing circular island demonstrate that the method is stable, efficient, and accurate enough to simulate the growing of epitaxial islands over a sufficiently long time period.

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PP3

Multi-Scale Modeling and Electrokinetic Techniques in Sediment Acoustics

We detail one approach to mapping between microscopic fields, which describe fluid and grain motion, and macroscopic fields, which characterize the volume-averaged material and its dynamics. Laboratory techniques were developed to make use of the fact that fluid motion is affected by grain surface chemistry at the microscopic level; this yields a coupled (macroscopic) electrokinetic-Biot theory. Since saturated, unconsolidated sediments exhibit this behavior, there is strong evidence for using poroelasticity in ocean sediment acoustics.

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PP3

On a Class of Young Measures Arising in the Nonlinear Membrane Theory

A nonlinear membrane model accounting for the density of bending moments is derived in terms of a special class of Young measures. A complete characterization of this class is provided.

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PP3

Nonlinear Isotropic Composites ?

We consider the class of sequentially laminated composites with nonlinear behavior of the constituting phases. Exact expressions for the effective stress energy potentials of two-dimensional composites are introduced. These allow to determine the stress potentials of rank-N sequentially laminated composites with arbitrary volume fractions and lamination directions. The effective response of composites with a power-law behavior of the phases is determined. It is demonstrated that as the rank of the lamination becomes large the behaviors of certain composites tend to be *isotropic*. The behaviors of these nearly isotropic composites are in agreement with corresponding second order estimates.

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PP3

Nano-Composite Material Properties: Homogenization over Flow-Induced Orientational Distributions

We report results of our research group on modeling the pipeline of nano-composite, nematic polymer materials. Highly anisotropic molecules are added to traditional polymeric materials to enhance properties. Current methods assume a random distribution of spheroidal molecules in a matrix, which is never the case. These materials are flow processed, and even homogeneous samples at very low concentrations acquire molecular orientational distributions. We have developed theory, analysis, and numerical bifurcation tools to characterize the pdf of the Doi-Hess kinetic theory for flow-processed nematic polymers. We report results of homogenization over monodomains of flow-induced nano-composite distribution functions, and quantify the effect of processing on nano-composite properties.

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PP3

Motion of Contact Line of a Crystal Over the Edge of Solid Mask in Selective Area Epitaxy

I will describe the model that allows for direct tracking of the homoepitaxial crystal growth out of the window etched in the solid, pre-deposited layer on the substrate. The growth is governed by the normal (to the crystal surface) flux from the vapor phase and by the surface diffusion. The model accounts for possibly non-uniform energy of the mask-vapor interface and for strong anisotropies of crystal surface energy and kinetic mobility. The results demonstrate that pinning of the contact line occurs as the radius of curvature of the mask edge approaches zero.

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PP3

Optimum Definition of Metal Tests Mechanical Properties (statistical Approach)

Now these properties control is sampling. Test number in standards is not proved. Control plans like Mil-Std-414 use lead to a great quantity of tests. It is unacceptable due to their labour input. Optimum plan definition is a nonlinear programming model and presents the tests number minimization for given control reliability. A priori information use allows to get the decision with tests small number. An example is given.

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PP3

On Multiscale Coupling in Polymer Fluids

In this talk, I will discuss models involving coupled effects from multiple scales. They will be formulated in a uniform energetic variation framework. In particular, we will present some analytical results for the dumbbell models, such as the global existence of classical solutions. Such models are also closely related to the viscoelastic materials.

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PP3

On the Application of Thomas and Poisson Branching Point Processes to Triboemission

The frequency distribution of triboemitted electrons from the abrasion of ceramic surfaces has been analyzed in terms of a modified Poisson distribution by Molina (Virginia Tech, PhD thesis) and by Molina et al. (Wear 255, 2003, 686-694). This distribution will be discussed in the context of the Thomas' (Biometrika 36, 1949, 18-25) distribution for "spatial" random variables that was extended by Matsuo et al. (J. of Math Phys. 25, 1984, 2174-2185) for "limited-length time windows".

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PP3

Numerical Study of Transitions in Nematics

We numerically investigate transition phenomena for steady state plane shear flows in nematics in the presence of external electric fields. The role of material properties, and the external electric field strength is analyzed. We study 8CB (4–n–octyl–4′–cyanobyphenyl), a "typical nematic polymer", and the small–molecule MBBA (4–methoxybenzylidene–4–n–butylaniline).

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PP3

Modeling Wetting and Spreading in Reactive Systems

In an effort to better understand the spreading of liquid solder on various metalizations, mathematical modeling is used to study wetting, spreading and dissolution for the configuration of a liquid metal drop on a metal substrate. Here, existing models have been employed to study the im-

portant physical regimes in the overall reactive spreading process. In particular, a modified solute transport model is used to study the wetting and dissolution behavior for an axisymmetric drop configuration. The isothermal model includes solute diffusion in the liquid drop, capillarity and a simple treatment of the spreading flow. The evolution of both the liquid-gas interface of the drop and the liquid-solid interface on the substrate are computed as the drop spreads. The boundary condition used to treat the liquid/solid/vapor contact line is an important aspect of the model.

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PP3

Misfits in Two-Dimensional Laminated Polycrystals

We study the deformation-induced martensitic transformations in a laminated polycrystalline material. We model the polycrystal as a domain $[0,1] \times [-L, L]$ with a finite number of rectangular grains $[k/n, (k+1)/n] \times [-L, L]$, and determine crystal's texture of each of the n grains by Bernoulli trials. The sequence of Bernoulli trials determines 3^n admissible configurations. The martensitic transformation is modeled as the solution to a global minimization problem of the linear elastic misfit energy among all admissible configurations. As $n \to \infty$, we determine the probability distribution of the minimizers in three cases: infinitely long grains $L = \infty$, asymptotically long grains $L \gg 1$, square grains $L = 1/n$.

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PP4

The Effect of Tri-Junction Conditions in Droplet Solidification

We carry out numerical simulations of solidification of a two-dimensional liquid droplet cooled at a point with different conditions at the tri-junctions where the solid, liquid, and gas phase meet. The velocity of the advancing solidification front is determined from the quasi-steady heat conduction equations in both solid and liquid phases. The singularity in heat flux at the tri-junction encountered in the previous studies is shown to disappear when kinetic undercooling and the Gibbs-Thomson effect at the solid-liquid interface are taken into account. Locally regular solutions can be obtained for arbitrary values of the contact angles at the tri-junction. The solidification rate and shapes of solid particles are studied as functions of the surface tension, the contact angles, and the thermal conductivities of the two phases. Higher solidification rates are found for lower surface tension and larger solid-to-liquid conductivity ratio. In the final stages of solidification a corner or cusp is formed in the shape of the solid in agreement with related experimental observations. The corner angle is decreased when the solid-to-liquid density ratio is decreased.

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PP4

Rank Three Laminates Are Almost Optimal for 2-D Diffusion

Given two starting materials in fixed volume fractions, one isotropic and the other anisotropic regarding heat diffusion, a region of laminates of rank at most three is created, which, if the starting material has a moderate degree of anisotropy, gives a very good approximation of the optimal bounds, one of which uses a coated disks construction. We also study the stability under homogenization of this region, to show that it can not be easily enlarged.

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PP4

Time Reversal Numerical Simulations for Randomly Layered Media

Via numerical simulation, we analyze waves propagating in complex one-dimensional media using a frequency domain formulation. We reproduce the time-reversal self-averaging effect which takes place in the presence of randomly varying layers. This is done in the regime where the inhomogeneities are smaller than the incident pulse, which propagates over long distances compared to its width. We show numerical evidence for possible use of a windowed time-reversal technique for detecting anomalies buried in the medium.

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PP4

Oscillatory Pattern Formation in a Driven Binary Immiscible Fluid

Via a coarse-grained model, we simulate dynamics of a binary immiscible fluid driven through the three dimensional microchannel. As an initial conditions, we have four parallel fluid streams of a checkerboard arrangement. We found that local perturbation in the inlet of the channel can cause creation of the oscillatory patterns where both fluids are intertwined. We analyzed stability of these patterns and the mechanism of the wavelength selection within the system.

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PP4

The Role of Shear in the Onset of the Bcc to Hcp Stress-Induced Martensitic Transformation in Iron

Iron shows a stress–induced martensitic phase transition from bcc to hcp, at pressures ranging from 9 to 16 GPa. Here we show that the transition pressure depends strongly on small amounts of shear deformation superimposed to the isotropic compressions. To this end, we construct a free–energy surface for Iron from quantum mechanics computations, as a function of the full deformation gradient. The onset of the microstructure is captured by using a sequential lamination algorithm.

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PP4

Simulation of Coarsening Faceted Crystal Surfaces: Dynamic Scalings, Correlations and Surface Statistics.

The hypothesis of dynamic scaling for the coarsening of a class of (micro-) faceted crystal surface models is considered. We present a novel numerical simulation scheme, based on a recent theory of Watson. Instances where the hypothesis holds and fails will be demonstrated through statistically significant studies of the evolving facet ensemble. The existence of correlation effects is also established to be generic, thereby eliminating one-point statistics as an effective closure scheme for the coarsening process.

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PP4

Universality of Scaling in Fracture

Scaling laws derived from mesoscopic discrete lattice models are typically used for coupling the mesoscopic damage evolution with the continuum damage response and in determining the size effects on the constitutive response of materials. However, simulations based on discrete lattice models can approach the continuum description only in the limit of infinite lattice system size, and hence numerical simulations on large system sizes are essential to represent progressive damage evolution in any realistic material. Unfortunately, numerical simulations based on lattice models are very time consuming and the maximum lattice size that can be simulated using the currently available computational power is well below the size required for coupling the mescoscopic lattice simulations to continuum damage evolution. Hence, accurate scaling laws are essential for describing damage evolution across these length scales.
Progressive damage evolution leading to failure of disordered quasi-brittle materials has been studied extensively using fuse, spring and beam lattice networks. This study investigates the universality of the scaling exponents when large fuse, spring and beam lattice networks are used for simulating the progressive damage evolution leading to fracture in quasi-brittle materials. Both triangular and diamond-type lattice topologies are considered. In this study, we consider a random threshold model problem, where all the bonds in the lattice network have the same stiffness (conductance for fuse model), and the initial micro-structural disorder is accounted for by sampling the bond breaking thresholds based on a uniform statistical distribution between 0 and 1. Based on the numerical simulations that span two orders of length scales and different lattice topologies, we investigate the universality of scaling laws in fracture.
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PP4

State-of-the-Art Optimization Techniques for Electronic Structure Calculations

The high cost of function evaluations in electronic structure calculations usually prevents the use of standard techniques to solve the associated optimization problems. Therefore, more sophisticated approaches are necessary. We will describe space-mapping optimization methods for these problems and present preliminary results.

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Topological Complexity and the Dynamics of Coarsening

We study the evolution of topologically complex two-phase mixtures during coarsening using a three-dimensional phase-field model . Applying this model to compute the curvature tensor as a function of position along the interface we propose a method for qualitative analysis and prediction of its evolution during coarsening. Also we compare the measured 3-D interfacial morphology after long coarsening times with that simulated numerically by the 3-D phase-field model.

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Surface and interface effects in solid films.

We considered a continuum model for evolution of epitaxially strained dislocation-free solid film. We derived a diffusion potential within a framework of small deformation taking into account the surface stress and the presence of the wetting layers. We found that due to a nonzero surface stress the film, unstable due to lattice mismatch, is affected differently for a film under compression than for one under tension. The magnitude of this effect depends on the relative stiffness of the film to the substrate. The presence of a wetting layer has the capacity to substantially stabilize the planar film.

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Phase-Field Approximations for Step-Flow Models

We present diffuse interface approximations for a step flow model in epitaxial growth. In this model the motion of step edges of discrete atomic layers is determined by the time evolution of an introduced phase-field variable. In order to incorporate the attachment-detachment kinetics at step edges as well as edge-diffusion into the phase-field model a degenerate mobility-function is established. The method of matched asymptotic expansion is used to show the recovery of the classical Burton-Cabrera-Frank equations for vanishing interfacial thickness.

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Regularized Anisotropic Mean Curvature Flow of Curves

The evolution of interfaces is of great importance for many physical processes, including phase transitions, epitaxial growth and grain boundaries. If the evolution is essentially interface-controlled; i.e. independent of the behaviour of the adjacent bulk phases the classic theory due to Mullins is today known as mean curvature flow

$$v = -\kappa, \tag{1}$$

where v is the scalar normal velocity and κ the curvature. This is a second order parabolic partial differential equation, which is intensively studied since its derivation. A

generalization that encompasses anisotropy read

$$\alpha v = -(\gamma + \gamma_{\phi\phi})\kappa, \tag{2}$$

with $\alpha(\phi) > 0$ a kinetic coefficient, $\gamma(\phi)$ the interfacial free energy density and ϕ the angle from a fixed axis to $\vec{n}$ the unit normal of the interface. If $\gamma(\phi)$ is convex, this equation is parabolic and well behaved. But crystalline materials are often endowed with interfacial energies which are not convex. Such energies lead to the possibility of corners, facets and wrinklings and turn the equation into a backward parabolic equation within nonconvex ranges of ϕ. One way to overcome this inherently unstable behavior in these ranges is to regularize the equation by allowing the energy to depend on curvature. Such a curvature dependence was already proposed on physical grounds by Herring. The theory of mean curvature flow based on a curvature dependent energy was introduced in Gurtin et al. When the interfacial free energy density has the specific form

$$\gamma + \frac{1}{2}\epsilon\kappa^2, \tag{3}$$

with $\epsilon > 0$ constant, the theory lead to the evolution equation

$$\alpha v = -(\gamma + \gamma_{\phi\phi})\kappa + \epsilon\left(\Delta_S\kappa + \frac{1}{2}\kappa^3\right) \tag{4}$$

which is fourth-order parabolic. We will derive, from a semi-implicit time discretization, a variational finite element formulation based on parametric finite elements. This algorithm allows the use of standard linear finite elements, only requiring continuity of the discrete functions. Furthermore the coarsening behaviour of this equation will be studied.

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Surface-Directed Spinodal Decomposition in a Stressed Thin Film

Two- and three-dimensional simulations of the spinodal decomposition of self-stressed, binary thin films using a Cahn-Hilliard model are presented. Two different sets of mechanical boundary conditions are considered, and compositional strains for a cubic-anisotropic system are treated. A composition-dependent interaction energy is assumed at the free surface. Numerical solution of the coupled Cahn-Hilliard and elastic equilibrium equations are obtained using an efficient nonlinear multigrid method. Results of simulations show that, for large enough compositional strain, surface-directed decomposition occurs at the traction-free surface, even when there is negligible surface interaction energy initially attracting one of the components. This decomposition is controlled by elasticity, and results in a local alignment of phases perpendicular to the free surface, in contrast to the parallel alignment produced by surface energy in stress-free systems.

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PP4

Solitary Waves in Layered Nonlinear Media

We have found numerical evidence that longitudinal elastic strain waves in a one-dimensional, periodically-layered, nonlinear medium can exhibit soliton-like behavior. Dispersion caused by reflections due to impedance mismatches at the interfaces, and nonlinear stress-strain relationships lead to this kind of behavior. We derive a homogenized system of equations and show that they agree well with direct solutions of the hyperbolic conservation laws using a high-resolution finite volume method.

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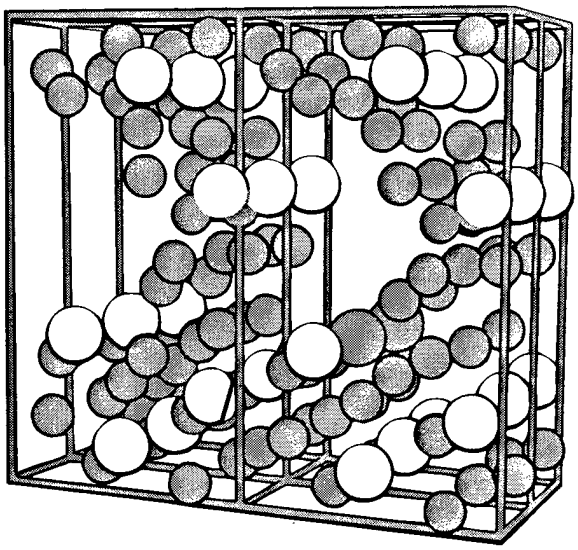

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